I. Abstracts

I. Oral Presentations

O1

Incorporating a two-electron density functional into the two-electron density matrix cumulant

Josh Hollett, Gurleen Cheema, Ernesto Cruz Velázquez, and Caio Correia

The University of Winnipeg

An accurate model of electronic structure, within the framework of cumulant functional theory, that combines density matrix functional theory and a two-electron density functional is proposed. The approximate parameterization of the two-electron density matrix (2-RDM) is designed to treat so-called potential dependent correlation. Whereas, the two-electron density functional (TDF) is designed to capture the short-range component of so-called universal correlation. Parameterization of the 2-RDM involves including the leading-order terms that contribute to inter and intra-pair correlation while satisfying constraints of N-representability. A TDF allows for the precise accounting of all energetic consequences of any proposed electron-electron interaction ansatz (*i.e.* kinetic, electron-electron potential and nucleus-electron potential). The advantages and challenges of such approaches will be discussed as well as preliminary results for atoms and small molecules.

O2

Quantum machine learning for data-driven coupled-cluster scheme

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This presentation will introduce the development of a data-driven coupled-cluster (DDCC) approach that integrates quantum machine learning (QML) with molecular electronic structure calculations. Our approach is built around a quantum–centric framework where quantum computing resources are utilized to predict coupled-cluster excitation amplitudes. These amplitudes are conventionally expensive to obtain through iterative coupled-cluster solvers and are central to the accurate computation of ground state molecular energies. In our work, wavefunction derived descriptors are used as input features to QML models, such as parametrized quantum circuits and quantum kernel based models, either allowing a full bypass of solving the amplitude equations or enabling the use of QML predicted excitation amplitudes as warm starts for the iterative solvers. In this presentation, I will discuss our investigations into the learning of parametrized quantum circuits and quantum kernels for the task of accurately predicting these excitation amplitudes, along with results on the transferability of the QML models assessed by their ability to predict excitation amplitudes for out-of-distribution molecular systems. These results will highlight the potential of QML models in the broader context of a hybrid quantum–classical pipeline for quantum chemistry.

O3

Molecular Electrostatics Through the Lens of Atoms: Development of Variational Hirshfeld Methods

Farnaz Heidar-Zadeh

Queen's University

It is common to use the electron density to partition a system into atomic regions. The necessity for such a partitioning scheme is rooted in the unquestionable role of atoms in chemistry and chemical modeling. Nevertheless, atomic properties are not well-defined concepts within the domain of quantum mechanics as they are not physical observables. One of the most popular families of atoms-in-molecules models is the Hirshfeld partitioning scheme. The various flavors of the Hirshfeld scheme mainly differ in choosing the reference proatom density that is being used to define the fuzzy atomic densities. To address the ambiguity in selecting the reference proatom density, we introduce new methods for computing atomic densities within the additive variational Hirshfeld framework, in which the proatom density is defined as a convex linear combination of spherically averaged charged atomic electron densities. We focus in particular on dipole- and charge-constrained variants and evaluate their performance on chemically diverse datasets, with emphasis on reproducing electrostatic potentials, molecular moments, and electrostatic interactions. Our ultimate goal is to improve force-field models.

O4

Quantum states of collections of confined molecules

Pierre-Nicholas Roy

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Confining molecules within nano-cavities like fullerenes quantizes their translational motion while preserving well-defined rovibrational states. The resulting structures, termed endofullerenes—with H2O@C60 being a prominent example—can be assembled into larger architectures such as carbon nanotubes, producing endofullerene ”peapods.” Within these assemblies, polar molecules couple through dipole-dipole interactions. The interplay between interaction strength and the spacing of monomer rovibrational levels can drive the system from a disordered to an ordered phase, a transition known as a quantum phase transition (QPT). Such a transition has recently been predicted for one-dimensional water [1,2]. We will discuss several computational tools for investigating these confined molecular chains. The first is the density matrix renormalization group (DMRG), and we will outline its capabilities for treating confined rotors [3,4]. For systems beyond one dimension, Path Integral Monte Carlo (PIMC) methods become more suitable, and we will present results obtained using discretized Gibbs sampling PIMC [6,7]. Finally, we will examine the conditions under which water chains can exhibit ferroelectric behavior.

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[6] M. S. Moeed, T. Serwatka, and P.-N. Roy, Pair Approximating the Action for Molecular Rotations in Path Integral Monte Carlo. J. Chem. Phys. 162, 024113 (2025).

[7] W. Zhang, M. S. Moeed, A. Bright, T. Serwatka, E. De Oliveira, and P.-N. Roy, Path integral Monte Carlo in a discrete variable representation with Gibbs sampling: dipolar planar rotor chain. J. Chem. Phys. 162, 014106 (2025).

O5

Activation of Small Molecules by Collisions with Gas Phase Transition Metals Ions

Hua Guo

University of New Mexico

The activation of small molecules, such as H2, CO2, and CH4, plays an important role in heterogeneous catalysis. Recently, there is significant interest in single atom catalysis (SAC), in which atomically dispersed transition metals are used to catalyze reactions. While it is well established that the surroundings of the single atom metal site play a pivotal role in catalysis, few studies have explored the effect of spin on catalysis. To this end, the study of spin-specific reactivity of transitions metal ions in gas phase collisions provides a unique and informative means to understand SAC, particularly the influence of spin. In collaboration with experimentalists, we carried out detailed dynamics studies of such reactions using first principles based full-dimensional potential energy surfaces.1-3 It is shown that intersystem crossing between different spin states plays a key role in reactions kinetics and dynamics.

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2. Liu, Y.; Ončák, M.; Meyer, J.; Ard, S. G.; Shuman, N. S.; Viggiano, A. A.; Guo, H. Multistate dynamics and kinetics of CO2 activation by Ta+ in the gas phase: Insights into single-atom catalysis. J. Am. Chem. Soc. 2024, 146, 14182-14193.

3. Liu, Y.; Ončák, M.; Lewis, T. W. R.; Meta, M.; Ard, S. G.; Shuman, N. S.; Meyer, J.; Viggiano, A. A.; Guo, H. Insights into facile methane activation by a spin forbidden reaction with Ta+ ions in the gas phase. Chem. Sci. 2025, 16, 5007-5016.

O6

Automatic construction of tree tensor networks for molecular quantum dynamics

Simon Neville

National Research Council Canada

Tree tensor network states have emerged as a powerful framework for the simulation of the quantum dynamics of molecules following photo-excitation. Here, a high-dimensional coefficient tensor representing the quantum state is represented by a hierarchical network of contractions of small-dimensional tensors, generating tree topologies. There exists great flexibility in the tree topology, allowing for a tailoring to the physical process being simulated. However, the computational cost is closely tied to the tree topology, and traditionally this had to be designed by hand on a system-by-system basis: a non-trivial task.

In this presentation, I will discuss an approach to automating the tree topology construction via the combination of ideas from quantum information theory and computer science. Specifically, I shall show how the mutual rate of entanglement of vibrational and electronic degrees of freedom can be combined with hierarchical clustering algorithms to reliably, rapidly, and fully automatically generate good tree topologies that are tailored to a given photo-induced molecular process.

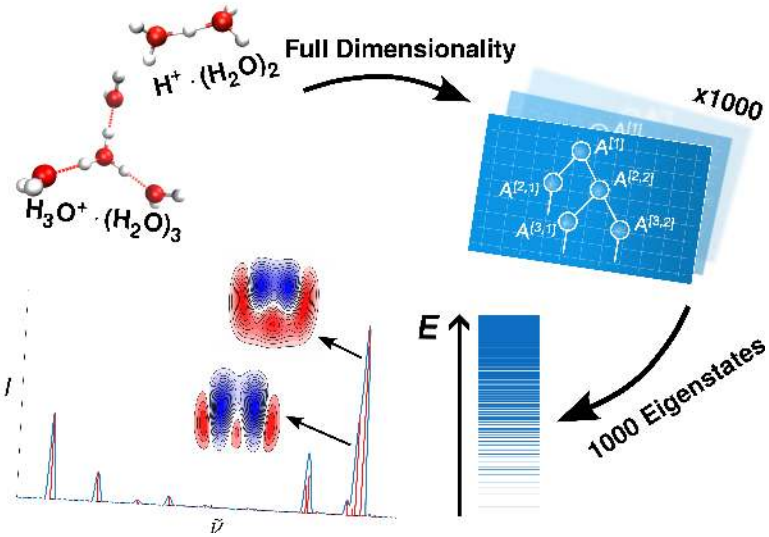
O7

Rigorous computation of thousands of vibrational states using tensor network methods

Henrik R. Larsson

University of California, Merced

Tree tensor network states (TTNSs) combined with the density matrix renormalization group (DMRG) are emerging as powerful tools for vibrational and vibronic structure simulations in molecules with strong coupling and fluxionality. In this talk, I discuss how TTNS methods enable accurate, full-dimensional computations of thousands of eigenstates for molecular systems ranging from quartic-force-field benchmarks to molecules with strong vibronic coupling and protonated water clusters as large as the 33-dimensional Eigen ion, $H_3O^+ \cdot (H_2O)_3$. I will show that for a widely used benchmark system, DMRG algorithms can boost the number of computed states by a factor of five compared to other methods, while simultaneously increasing the accuracy by two orders of magnitude. Finally, I will show how to directly target excited eigenstates for these systems.



O8

Thermalization of a quantum circuit

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Solution methods on the quantum computer often have misleading computational complexity. For example, wavefunction preparation can be very costly, eliminating quantum advantage or the ability for the quantum computer to outperform all classical methods. A curious feature of quantum systems is that the thermalize, or achieve an equilibrium statistical ensemble value after a long-time. This is known as thermalization and it is well understood that this occurs in classical systems. In quantum mechanics, we suppose that thermalization also occurs in some systems. Using thermalization can provide an equal superposition of eigenstates in a time-average. Using the quantum phase estimation subroutine on the quantum computer allows for a weighting of the eventual expectation value that appears to be applicable in a wide variety of cases. This strategy circumvents the need for wavefunction preparation on the quantum computer. I discuss the implication of allowing a quantum circuit to thermalize and how to use it in a variety of use cases.

This research was undertaken, in part, thanks to funding from the Canada Research Chairs Program (CRC-2021-00257). This work has been supported in part by the Natural Sciences and Engineering Research Council of Canada (NSERC) under grants RGPIN-2023-05510 and DGECR-2023-00026.

O9

Conserving non-Abelian symmetries with quantum computing

Ryan J. MacDonell

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The steady advance of quantum technologies in recent years has brought their application to quantum chemistry to the forefront of research. Most quantum algorithms for quantum chemistry work by expressing the Hamiltonian in a basis of qubits and fragmenting the Hamiltonian into individual qubit operations. The product of exponentials of these operations then approximate the exponential of the Hamiltonian. However, random orders of fragments generally break symmetries of the Hamiltonian, such as spin and spatial symmetry. Abelian symmetries are local in a single-particle, symmetry-adapted basis and can thus be easily restored by grouping fragments. We show that the same strategy cannot restore non-Abelian symmetries. We demonstate an alternate approach whereby non-commuting terms can be projected out of a symmetry-conserving operator and rotated into a set of commuting terms such that they are exactly exponentiated and symmetry is conserved. Finally, we show the consequences of symmetry conservation for quantum chemistry. Symmetries have an exponential advantage for classical computers relative to quantum computers, enabling large-scale tests of quantum algorithms while the technology develops.

O10

The Dynamic World of Nucleic Acids: Lessons from Multiscale Computational Chemistry

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Nucleic acids are the most basic molecules of life, storing and transmitting genetic information in all living organisms. To enhance nucleic acid programmability, stability, and function, the fundamental building blocks of DNA and RNA are commonly modified. Furthermore, the ease of synthesis of nucleic acids functionalized at any nucleobase, sugar, or phosphate site, as well as the ability of modifications to impact base pairing, chemical stability, conformation, and interactions with proteins, has led to the development of a wealth of unique modifications with far-reaching applications from drugs and vaccines to nanomachines. Unfortunately, the lack of known structure–function relationships for a range of modified nucleic acids raises questions such as how modifications improve organism survival and how modifications can be used to their full potential in medicine and biotechnology. Computational chemistry provides a valuable tool to gain insights necessary to understand the chemistry of modified nucleic acid building blocks, serving as a powerful predictor of experimental outcomes and clarifying discrepancies between experimental hypotheses and results. This talk will highlight research conducted by high school students, undergraduate students, graduate students, and postdoctoral fellows that uses a range of computational techniques to shed light on the biological implications and design of modified nucleic acids.

O11

Adiabatic Populations in High Dimensionality Quantum Simulations using Matrix Product State Sampling

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Non-adiabatic dynamics is central to photochemistry, energy transfer, and electronically excited-state processes, but its interpretation depends strongly on the electronic representation. Tensor-network quantum dynamics uses a diabatic basis, but many important observables — and comparisons to mixed quantum-classical methods — are natural in the adiabatic basis. Directly adiabatising a high-dimensional wavefunction is infeasible: the transformation is a strongly geometry-dependent, high-rank object that cannot usually be represented compactly as a tensor operator. As a result, adiabatic observables have been difficult to obtain, even approximately.

Here, we introduce a sampling-based route to adiabatic observables from matrix product state wavefunctions. By adapting the sampling approach of Ferris and Vidal (A. Ferris & G. Vidal, Phys. Rev. B, 2012, 85), nuclear configurations are drawn efficiently from the density, and the local electronic wavefunction is then transformed. This bypasses the full adiabatisation of the wavefunction or any global fit of the transformation, and the resulting estimator is efficient, unbiased, error-bounded, requires no Markov chain, and suitable for generic Hamiltonians. We demonstrate the method on 24-dimensional pyrazine and a 78-dimensional BMA radical cation model, revealing large differences between diabatic and adiabatic population dynamics. More generally, this approach can be used to perform analysis on wavefunctions using tools normally reserved for trajectory-based methods, opening new avenues for understanding high-dimensional quantum simulations.

O12

Exact Exchange in Orbital-Free Density-Functional Theory

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We show that the Fermi–Amaldi functional is the exact exchange functional within the orbital-free Levy–Perdew–Sahni (LPS) equation for the square root of the electron density. This result follows from a reinterpretation of the LPS scheme based on a reference system of non-interacting boson-like fermions occupying a single spatial orbital. In contrast to the orbital-dependent Kohn–Sham exact exchange, the exact LPS exchange is explicitly multiplicative and fully compatible with the orbital-free formalism. Self-consistent calculations for atoms and molecules demonstrate improved accuracy relative to conventional LPS approximations. These findings provide a foundation for incorporating exact exchange and hybrid-functional concepts into the orbital-free LPS framework.

O13

A First-Quantized Real-Space Grid Representation of Electronic Structure on Quantum Computers

Amir Ayati, Omid Tarkhaneh, Ehsan Ghasempouri, and Stijn De Baerdemacker

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A central challenge of quantum simulation of electronic structure is choosing a representation that scales gracefully with system size while remaining compatible with both near-term variational and fault-tolerant phase-estimation algorithms. Standard second-quantized formulations require $\mathcal{O}(N)$ qubits and $\mathcal{O}(N^4)$ two-body matrix elements for N basis functions, whereas real-space first-quantized representations need only $\mathcal{O}(\eta \log_2 m)$ qubits for η electrons on an m-point mesh, with a diagonal electron-electron interaction operator.

We propose a first-quantized real-space mesh as a natural representation of the electronic structure of atoms and molecules on a quantum register. Position and shift operators on the discretized configuration space are expressed directly as Pauli words on $w = \log_2(m)$ qubits per axis per electron, the kinetic operator becomes a Hermitian-symmetrized finite-volume Laplacian, and electron-nuclear and electron-electron interactions remain diagonal in the position basis. The representation scales favourably with both spatial resolution and particle number, supports fermionic antisymmetrization, and accommodates non-uniform grids that concentrate resources near the nuclei.

We then present three complementary algorithms implemented on top of this representation – variational ground-state preparation (VQE), real-time evolution via Strang-split Trotterization, and single-ancilla iterative phase estimation – and benchmark them on the hydrogen and helium atoms.

O14

The Scientific Legacy of Axel Becke

Andreas Savin

Laboratoire de Chimie Théorique, CNRS and Sorbonne University, Paris, France

In science, important ideas act like seeds: they give birth to new domains, that were not apparent in the original work where the ideas showed up. Papers by Axel Becke have this potency. Two examples are given:

• the electron localization function (ELF), and

• the justification of hybrid methods using the adiabatic connection in density functional theory (DFT).

The first one was adopted by people like Reinhard Nesper and Yuri Grin leading to new path in experimental chemistry. The second one could be used in something seemingly distant from DFT: the correction of basis set errors.

O15

TBD

Gershom (Jan M.L.) Martin

Weizmann Institute of Science, Rehovot, Israel

O16

Axel Becke: Reminiscences and two of his greatest hits

Kieron Burke

UC Irvine

Axel Becke was one of the most influential figures in the history of modern density functional theory (DFT). At a pivotal moment in the late 1980s and early 1990s, his remarkable physical intuition and deep understanding of electronic structure transformed the field and helped establish DFT as the dominant electronic structure method in chemistry. The impact of his work continues to be felt across chemistry, materials science, and condensed-matter physics.

In this memorial lecture, I will share personal reminiscences of Axel, reflecting on his unique scientific style, his generosity of spirit, and the profound influence he had on my own career and on generations of researchers. I will focus on two of his most important contributions: the B88 generalized gradient approximation for exchange and the introduction of hybrid functionals that combine density functional approximations with Hartree–Fock exchange. These innovations not only revolutionized practical electronic structure calculations but also shaped the direction of DFT research for decades. Even today, they remain central to the development of new functionals and to our understanding of the strengths and limitations of electronic structure theory. Through these examples, I hope to convey both the brilliance of Axel's scientific contributions and the enduring legacy he leaves to our community.

O17

There is no substitute for good physics: Performance of minimally empirical density-functional approximations for molecular benchmarks

Erin Johnson

Department of Chemistry, Dalhousie University

In this talk, I will present results from minimally empirical dispersion-corrected hybrid functionals for the GMTKN55 benchmark. Notably, replacement of the Becke-Johnson damping function with a new damping function dependent on atomic number, proposed by Becke in his last scientific paper, results in more consistent reliability. Accuracy can be further improved through construction of corresponding local-hybrid functionals.

O18

Mean Fields Can (Sometimes) Be Exact: Going Beyond the Hohenberg-Kohn Theorem

Paul Ayers

Department of Chemistry and Chemical Biology; McMaster University

Traditionally highly-accurate numerical solutions to the quantum many-body problem have high computational cost and low interpretability, hindering their applicability and utility for (bio)chemical problems, where systems are large and extracting conceptual insight to guide experimentalists is of paramount importance. In this talk, I'll explain how every quantum system can be exactly described using a (possibly symmetry-broken) product wavefunction with a finite number of factors. This gives an interpretable mean-field description and provides a systematic way to control the cost/accuracy trade-off in practical computations. This new twist on an old approach has special relevance in chemistry (because it reinforces the "electron pair picture") and quantum computing (because boson-product wavefunctions are described by the permanents of coefficient matrices). If time permits, I'll describe some related approaches, including "generalized DFT" methods, which fit into the same conceptual framework.

O19

Performance of Density Functionals for Cytochrome P450

H. Bernhard Schlegel[1] and Robert D. Bach[2]

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Cytochrome P450s (CYP) are a family of iron heme-containing mono-oxygenases that can catalyze the hydroxylation of non-activated C-H bonds. This is one of the more difficult chemical reactions to achieve, involving the insertion of one atom from molecular oxygen which is activated by a reduced organic heme- iron. The nature of the catalytic mechanism has been a subject of controversy for nearly fifty years. Most of the computational studies have used the B3LYP density functional, but this functional routinely underestimates barrier heights and bond dissociation enthalpies (BDE). The M06-2X functional has been used lately as it provides better BDE's, especially for peroxide O-O bonds. However, M06-2X can have difficulties for high spin states, particularly for transition metals. A recent study compared the performance of 250 density functionals in describing the spin states and binding energies for a number of porphyrin complexes. We have chosen representatives of the best functionals to examine key intermediates in possible reactions steps for cytochrome P450 oxidation reaction. Specifically, we have compared the ωB97XD, APFD, B3PW91, O3LYP, PBE1PBE and r2SCAN functionals with B3LYP and M06-2X. The best functionals appear to be ωB97XD, B3PW91 and PBE1PBE.

O20

Standing on Axel's shoulders: Some recent developments in density functionals

Martin Head-Gordon

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[2] *Chemical Sciences Division, Lawrence Berkeley National Laboratory, Berkeley CA 94720, USA*

It is a pleasure to help celebrate and remember Axel Becke, and particularly his pioneering contributions to the development of modern density functional theory. In this talk, I will try to do so by describing some recent developments aimed at improved density functionals from my group. None of this work would have been possible without Axel's inventions. In particular, seeking the broadest accuracy that is possible for hybrid density functionals, I will briefly summarize our new Carefully Optimized and Appropriately Constrained Hybrid (COACH). I will then discuss new work that aims to provide DFT calculations with error estimates, and show that transferable and useful error estimates can be obtained using statistical theory applied to generalized basis functionals (i.e. modern hybrids). These error estimates can also be applied to energy differences, and even differences of energy differences, to reflect the extent of error cancellation.

O21

Approaching more general solutions of density functional theory

Jing Kong

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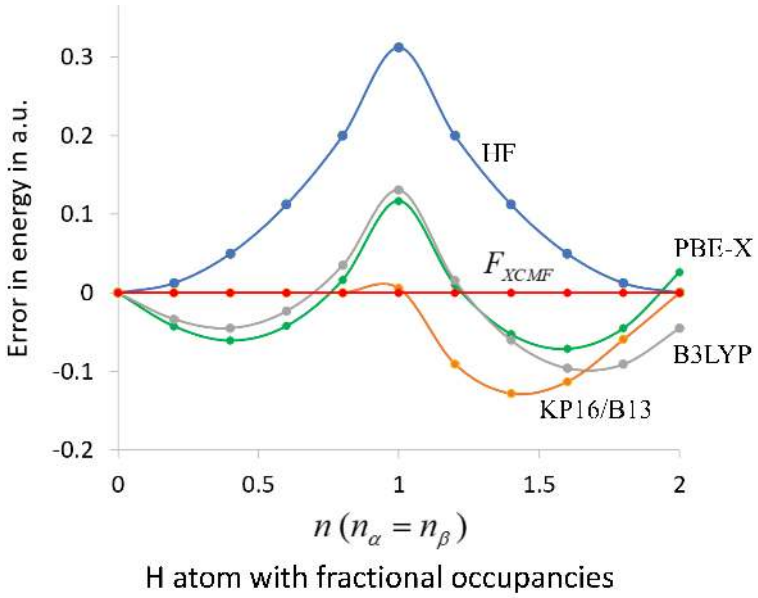
This contribution was initially motivated by Axel Becke's ingenious work on treating nondynamic correlation in density functional theory (DFT) [1]. Becke'03, '05 and '13 showed that the multireference character in electron correlation could be defined and treated with the single-determinant DFT, contrary to common beliefs. We modified the Becke'13 method by modeling the adiabatic connection for the correlation kinetic energy, resulting in a functional with far fewer parameters. The new functional, abbreviated as KP16/B13 [2], is not only capable of recovering the majority of strong correlations for extreme cases such as the dissociation of a covalent bond, but also competitive to contemporary heavily parameterized methods in standard benchmarking. The method was further extended to correct the charge delocalization error of DFT in some common cases.

Still, KP16/B13 was unable to handle general ensemble-representable densities. Indeed, some basic concepts related to that type of density, such as the locality, physical necessity of fractional charge, and v-representability, are still being debated. In this presentation, we argue that any physically reasonable density is ensemble v-representable within a finite accuracy [3,4]. We start from a hypothetical physical principle that defines molecules in a limited volume. The principle shows that all molecules are entangled in the number of electrons and leads to the possibility of fractional numbers of electrons. The universal v-representability admits the definition of an exchange-correlation functional for non-interacting ensemble densities. It is essentially equivalent to exact exchange for a single-determinant v-representable density and recovers most of the exchange-correlation effect for ensemble densities.



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O22

Remembering how Axel Becke impacted me and where I have taken that since

Stephen Dale

National University of Singapore

In science our impact is regularly measured by citation metrics and awards (among others), and there is no doubt that Axel was one of the all-time superstars in this respect. Less measurable, but even more important, is the impact we have on our colleagues and students that surround us. I believe Axel had a profoundly positive impact on the people around him, and I hope to spend my time in this presentation sharing some stories that reflect that.

I had the good fortune to be Axel's Postdoc from 2017-2019. This position with Axel allowed me to continue working on a DFT problem I had developed a fascination with, delocalisation error. Specifically, we revisited his B05 functional to show that it is capable of addressing some of the problems caused by delocalisation error.

This presentation will share samplings of the research profile I have developed since leaving his group. Highlights of these research topics will be:

- a new differentiable DFT program developed which hopes to address the difficulties of implementing a B05 convergence algorithm.
- new results on delocalisation errors and pitfalls to avoid.
- a new transition state searching algorithm.

O23

The In Silico Search for an Endogenous Anti-Alzheimer's Disease Compound

Donald Weaver

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[2] *Krembil Research Institute, University Health Network, Toronto, Canada*

The molecular pathogenesis of Alzheimer's disease (AD), humankind's most prevalent dementia, remains unknown; correspondingly, the role of β-amyloid (Aβ) peptide in the cause and progression of AD remains an issue of controversy and dispute – a dispute unresolved by decades of cellular levels studies. AD research needs an explicit atomistic/molecular-level understanding of Aβ and the role it plays in AD. We are endeavouring to achieve this understanding through extensive in silico modelling calculations (at quantum mechanical [DFT] and molecular mechanical levels) to enable "seeing the unseeable" events that unfold during the molecular mechanistic course of this devastating neurodegenerative disease.

Based on preliminary molecular dynamics simulations, we demonstrated that Aβ peptide monomer and oligomers, implicated in AD pathology, electrostatically bind via their cationic HHQK N-terminal segment to neuronal membranes followed by destructive membrane insertion of the C-terminal; we then demonstrated an identical membrane insertion into bacterial membranes, analogous to an immunopeptide. From these computational simulations, the following new molecular-level model of AD emerges: In response to pathogen/damage-associated molecular pattern stimulating events (e.g. infection, pollution, trauma), Aβ is released as a protective peptide exhibiting immunomodulatory and antimicrobial activities. Aβ's antimicrobial properties (whether or not bacteria are present) result in a misdirected attack upon 'self' neurons, arising from electrotopological similarities between neurons and bacteria in anionic charge geometries on outer leaflet membrane macromolecules (gangliosides in neurons; lipopolysaccharides in bacteria), rendering them similarly susceptible to membrane destruction. This constitutes a new mechanistic model of AD recognizing Aβ as a physiologically oligomerizing physiological peptide within a larger autoimmune conceptualization of AD.

Since immune processes are homeostatically regulated, there are endogenous control systems, offering druggable targets against immunopathic disease. To identify an endogenous "anti-AD" molecule, an in silico screen of 1137 brain molecules against Aβ membrane destruction was performed. This screen identified multiple metabolites of tryptophan and arginine as putative endogenous anti-AD agents. An extensive series of QM/MM and DFT calculations were then performed to explicitly model their mode of action in preventing Aβ-mediated neurotoxicity.

Based upon a comprehensive series of molecular modelling calculations (including molecular dynamics simulations, peptide homology modelling, in silico high

throughput screening campaigns, QM/MM and DFT docking studies) at molecular mechanics and molecular quantum mechanics levels of theory, new insights into the cause of AD have been deduced. These calculations suggest that AD is caused because the brain’s immune system cannot differentiate neurons from bacteria.

O24

From the correlation-factor model to the relation between correlation and the derivative discontinuity

Matthias Ernzerhof

Department of Chemistry, University of Montreal

The correlation-factor approach to exchange and correlation is based on a simple real-space ansatz in which the exchange–correlation hole is written as $\rho_{xc}(\mathbf{r}, u) = f_c(\mathbf{r}, u)\, \rho_x(\mathbf{r}, u)$ (6,7). Within this framework, the Becke–Roussel model (2) plays a central role because it provides a compact, non-oscillatory representation of the exchange hole that can be constrained through the on-top value, the curvature, the normalization, and the exchange energy per particle. In this way, it offers a flexible bridge between exact-exchange information and hole-based density-functional modeling, in the spirit of Becke's emphasis on real-space constructions of exchange and correlation, including his coordinate-space correlation model and his later real-space models for nondynamical, static, and strong correlation (1-5). In this contribution, we will give a short account of the correlation-factor model and of the way in which the Becke–Roussel construction underlies several of its developments, including extensions designed to incorporate exchange plus static correlation from multiconfigurational reference states. We will then turn to a broader viewpoint on correlation suggested by recent work (8): strong correlation and the derivative discontinuity can be understood within a common framework in terms of charge stiffness and the subdivision of Hilbert space into weakly communicating charge sectors. In this perspective, strong correlation corresponds to the suppression of collective charge fluctuations within a sector, whereas the derivative discontinuity appears as the non-analytic switching between competing sectors. Finally, we will discuss the role of the complex domain in mean-field electronic-structure theory (9). An approximate exchange–correlation functional $E_{\text{xc}}[\rho]$ can in principle generate stationary densities that are complex. This suggests that approximate density functionals possess a broader variational landscape than is usually assumed, with additional branches of self-consistent solutions that may carry physical meaning.

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O25

Graphical model reduction theorems that preserve qualitative behavior

Marc Roussel

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[2] *Department of Chemistry and Biochemistry, University of Lethbridge*

When developing models of biochemical reaction networks, we typically run into two problems: the network itself is somewhat uncertain, and many of the kinetic constants are unknown. Most biochemical modelling therefore involves the generation and testing of hypotheses in the presence of incomplete data. Often, the models are more elaborate than can be entirely justified by the data, but it is less than clear where models can be pruned. Qualitative stability analysis methods, often associated with graphical analyses, provide necessary conditions for models to have specified behaviours, such as oscillations or multistability. Accordingly, they can both identify the generator of a particular behaviour in a model and suggest what parts of the model are superfluous. Following a brief review of Ivanova's qualitative instability theorems, some theorems for model reduction based on this theory will be outlined and illustrated.

O26

Adventures and Challenges in the Non-Equilibrium Steady State

Paul Brumer

Chemical Physics Theory Group, Department of Chemistry, University of Toronto

Large numbers of natural and designed processes occur in the non-equilibrium steady state (NESS). Examples of the former and latter include retinal isomerization in vision, and donor-accepter complexes in energy transfer devices. Such systems present significant theoretical and computational challenges in open system quantum mechanics. We introduce this topic and discuss some developments in determining rates within networks, using quantum interference to control open system processes, and problems associated with limited experimental data. Time permitting, I will list some of the disturbing trends (in my view) in modern scientific approaches.

O27

Computational Methods for Degenerate and Non-Degenerate Two-photon Absorption

Alex Brown

Department of Chemistry, University of Alberta

Two-photon absorption (2PA) is a nonlinear optical process which requires a high light intensity and leads to the simultaneous absorption of two photons. The use of low-energy (near-infrared) focused light allows deeper penetration into the material or tissue being analyzed while causing less damage. Therefore, 2PA has widespread applications in microscopy, 3D data storage, microfabrication, bioimaging and photodynamic therapy. However, the design of efficient molecular light absorbers still poses challenges, and, as such, computational prediction of 2PA [1,2] can play an important role in understanding and predicting absorption properties of new synthetic targets. I will discuss our recent computational research examining two-photon absorption (2PA) cross-sections [1-4] in small fluorescent molecules and fluorescent protein chromophores. I will introduce 2PA including the use of two- (or few-) level models for interpreting 2PA cross-sections, based on transition dipole moments (oscillator strengths), permanent dipole moments, and excitation energies. I will also emphasize differences between degenerate 2PA, where both absorbed photons have equal energies, and non-degenerate 2PA, where absorbed photons have different energies. Results presented are determined using both time-dependent density functional theory (TD-DFT) and the approximate second-order coupled cluster (RI-CC2) approaches. I will show the importance of the choice of functional for predicting 2PA cross-sections [1] but also hioghlight alternative approaches such as GW/BSE [2].

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[4] I.A. Elayan and A. Brown, 2023, Degenerate and Non-Degenerate Two-Photon Absorption of Coumarin Dyes, Phys. Chem. Chem. Phys., 25, 16772-16780. DOI: 10.1039/D3CP00723E

O28

Frontier models are better at scientific research than I am

Isaac Tamblyn

University of Ottawa

In this presentation, I will argue and demonstrate that frontier models (e.g. 5.5 and 4.8) are better than I am at many aspects of research, including summarizing articles, coming up which student projects, writing code, writing and refereeing manuscripts, and generating ”insight”.

I will provide evidence for this and discuss the implications.

O29

Multiscale computational modelling of complex materials: from clay ion exchange to long-time-scale dynamics

Yalda Pedram[1], Yaoting Zhang[1], Scott Briggs[2], Chang Seok Kim[2], and Laurent Karim Béland[1]

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Canada's approach to deep geological repositories for nuclear waste relies on a multi-barrier system, including copper-coated steel containers surrounded by a bentonite buffer. The performance of bentonite is largely governed by montmorillonite (MMT), a negatively charged swelling clay stabilized by interlayer cations such as Na^{+} and Ca^{2+}. Copper corrosion products may interact with the clay and drive ion exchange, potentially altering the hydration, swelling, and mechanical response of the bentonite barrier.

To investigate these effects, we employ a multiscale computational approach. Density functional theory (DFT) simulations are first used to characterize Cu^{2+} interactions with MMT at the electronic and atomic scales. Molecular dynamics (MD) simulations then quantify the energetic and structural effects of Cu^{2+} exchange with native interlayer cations, including changes in layer spacing, swelling behaviour, hydration structure, and ion mobility. To extend the modelling framework beyond the atomistic scale, we also develop mesoscale clay platelet models, in which physically motivated interaction terms are combined with Gaussian process regression (GPR) corrections to predict larger-scale swelling and mechanical behaviour under different environmental conditions. This framework bridges atomistic interactions and mesoscale bentonite properties, providing a predictive approach for modelling the swelling and mechanical behaviour of clay-based engineered barriers.

Also discussed is the ongoing work on pyKMC, a Python framework for adaptive off-lattice kinetic Monte Carlo simulations, as a route to access longer-time-scale structural evolution in materials beyond the timescales accessible to conventional molecular dynamics.

O30

Covalent: Interpretable Collective Variable Discovery with Geometric Comparison of Learned CV Spaces

Myongin Oh

Department of Chemistry, Memorial University of Newfoundland, St. John's, NL, Canada

Identifying collective variables (CVs) that are both discriminative and interpretable remains a central challenge for enhanced sampling and mechanistic analysis of chemical systems. We present Covalent (Collective variables learnt by a computer), a supervised machine learning-based CV discovery pipeline that combines a filter-wrapper-substitution feature funnel with an improved, Riemannian-optimized variant of harmonic linear discriminant analysis (GDHLDA) and a post hoc subspace rotation to concentrate pairwise transition information. We demonstrate the distinguishability and interpretability of CVs generated by Covalent and its applicability across diverse systems, ranging from polycyclic aromatic hydrocarbons to membrane proteins. Beyond identifying low-dimensional CVs that separate metastable states, Covalent also provides geometric insight into how different linear CV spaces can be compared.

O31

Discovering physical behaviours with AI/ML: Choosing proper molecular descriptors and metrics

Mikko Karttunen

[1] *European Laboratory for Learning and Intelligent Systems (ELLIS) Institute Finland, Espoo, Finland*

[2] *Dept. of Technical Physics, University of Eastern Finland, Kuopio, Finland*

In this presentation, I will discuss artificial intelligence (AI) and machine learning (ML) based approaches to study structure and dynamics of soft materials [1,2]. Although the examples will be from soft and biological systems, the methods themselves are general and have broader applicability. The first example is lipids. Their phase behavior is complex, and even single component bilayers still pose challenges. The gel and fluid phases of lipid bilayers are planar and conformationally homogeneous, but the ripple phase, which exists at temperatures between the gel and fluid phases, undulates in an asymmetric sawtooth pattern and consists of heterogeneous conformational clusters. The ML approach here identifies the molecular conformations, and changes in their respective proportions that give rise to the changes. The method is also demonstrated for multicomponent systems.

References:

1. Elucidating Lipid Conformations in the Ripple Phase: Machine Learning Reveals Four Lipid Populations. Davies, Matthew; Reyes-Figueroa, A. D.; Gurtovenko, Andrey A.; Frankel, Daniel; Karttunen, Mikko. Biophys. J. 122, P442-450 (2023).

2. Learning glass transition temperatures via dimensionality reduction with data from computer simulations: Polymers as the pilot case. Glova, Artem; Karttunen, Mikko. J. Chem. Phys. 161, 184902 (2024).

O32

Long Range Interactions in Machine Learning Interatomic Potentials

Phuc Tu and **Christopher Rowley**

Carleton University

Machine-learned interatomic potentials have emerged as alternatives to molecular mechanical force fields. These models are trained on quantum mechanical data and can, in principle, match the accuracy of QM methods while remaining sufficiently fast to perform long-timescale MD simulations. To date, popular models have been effective at describing molecular species and single-component liquids. However, they are not always transferable to systems and configurations outside their training domain, and long-range dispersion and electrostatic interactions are not consistently included. Our group has developed a machine-learning implementation of the exchange-hole dipole moment model (MLXDM) to account for dispersion interactions within an MLIP. We have also implemented a fourth-generation, transferable neural network potential for bioorganic molecules composed of C, N, O, and H, incorporating long-range electrostatics via a machine-learning adaptation of the QEq charge-equilibration method. We compare this approach to a delta-learning strategy, in which a neural network corrects a tight-binding DFT method to match results from a full conventional DFT calculation.

O33

How Photosynthetic Proteins Control Energy Flow

Divya Matta Kaur

Brock University

Photosynthetic proteins convert light into chemical potential through coupled processes involving excitation, charge separation, electron transfer, proton movement, and changes in local hydration. These processes are not determined by cofactors alone; they are shaped by the surrounding protein matrix, which modulates electrostatics, solvent organization, and redox energetics. In this talk, I will discuss how hybrid computational methods and continuum electrostatic calculations can be used to probe the molecular factors that regulate energy flow in photosynthetic complexes. Our work examines how local protein environments influence charge localization, redox tuning, hydration networks, and proton-coupled processes that support light-driven function. By connecting structure, electrostatics, and energetics, this work aims to identify how photosynthetic proteins maintain functional efficiency across different molecular and energetic contexts. Understanding these principles is important not only for explaining how natural photosynthetic systems sustain efficient light-driven chemistry, but also for informing the design of bioinspired materials and molecular systems for energy conversion.

O34

Sodium channel interactions with tetrodotoxin and molecular determinants of selectivity

Anna Ananchenko, Sheyla Montero Vega, and Christopher Rowley

Carleton University

Voltage-gated sodium channels (NaVs) play an important role in the electric signaling of cells by allowing the movement of ions across cellular membranes in response to changes in membrane potential. The nine human NaV subtypes perform distinct physiological functions and are of substantial therapeutic interest due to their involvement in several physical conditions, such as neurological and cardiac disorders, as well as nociception. Many clinically relevant compounds target NaVs, including the pufferfish toxin tetrodotoxin (TTX), a highly potent and selective channel blocker with potential applications in neuropathic pain management. Despite their amino acid sequence being highly conserved, certain NaV subtypes, such as NaV1.6 and NaV1.7, are highly sensitive to TTX, with IC50 values in the nanomolar range, while others, such as Nav1.5 and NaV1.8 are resistant to TTX. Understanding the molecular mechanism for NaV-TTX selectivity is important for development of TTX-based pain therapies. Using recent cryo- electron microscopy structures of TTX-bound NaV channels, we use molecular dynamics (MD) simulations and free energy perturbation (FEP) to investigate the key molecular interactions which dictate TTX selectivity, comparing to experimental KD values. These insights establish a molecular basis for further developing TTX-derived compounds for pain therapeutics.

O35

When a Few Trees Dominate the Forest: Outlier Analysis on Thermochemical Benchmarks

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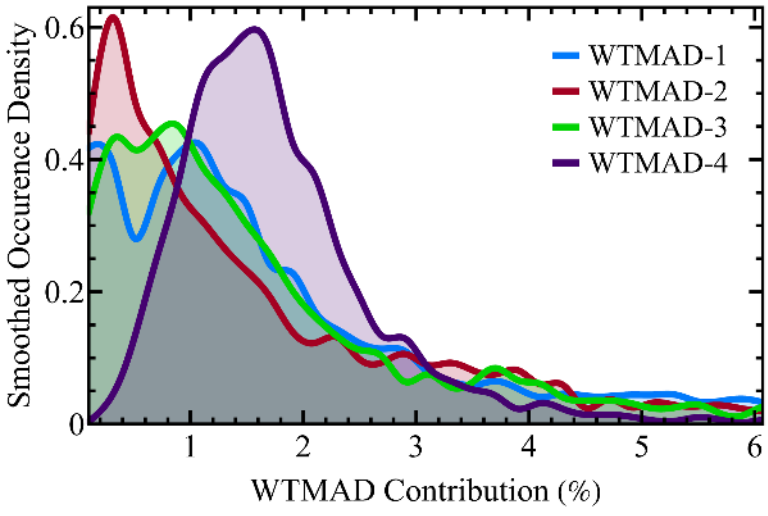
[2] *Department of Physics and Atmospheric Science, Dalhousie University, 6310 Coburg Road, Halifax, Nova Scotia, B3H 4R2, Canada.*

[3] *Yusuf Hamied Department of Chemistry, University of Cambridge, Lensfield Road, Cambridge, CB2 1EW, United Kingdom.*

The GMTKN55 data set is a collection of standard benchmarks in molecular quantum chemistry that spans small- and large-molecule thermochemistry, reaction barriers, and non-covalent interactions. The error across this collection of benchmarks is reported as a weighted mean absolute deviation (WTMAD). We identify a flaw in the canonical WTMAD definitions, which weight some benchmarks orders of magnitude more heavily than others, with the top 3 benchmarks contributing as much to the total WTMAD-2 as the bottom 36. A new WTMAD-4 metric is proposed, and assessed on hundreds of DFAs from the literature, including the DM21 and Skala machine-learned functionals that have garnered recent attention. We highlight literature examples where DFAs parameterized by minimising WTMAD-2 underperform on benchmarks marginalised by that metric, and perform outlier analysis for all functionals, providing insight into both performance and consistency across the dataset. We then test the exchange-hole dipole moment (XDM) dispersion correction (and many-body dispersion, MBD) in combination with minimally-empirical DFAs for the first time on GMTKN55. XDM shows excellent performance on both GMTKN55 and molecular crystals when paired with minimally empirical functionals such as revPBE0 and B86bPBE0 and Becke's recently proposed Z-damping function.



O36

Fast rational enzyme design via non-equilibirum alchemical transformations and ab-initio derived force fields

Carlos Castillo-Orellana[1], Esteban Vöhringer-Martinez[2], and Farnaz Heidar-Zadeh[1]

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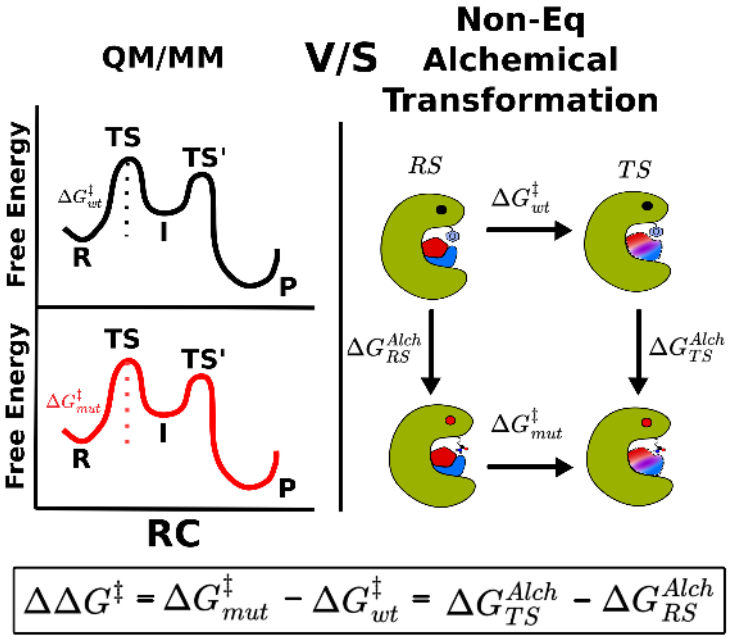
[2] *Departamento de fisicoquimica, Universidad de Concepcion, Chile*

Enzyme engineering is an increasingly important field in biotechnology, industry, and medicine. Traditionally, new enzymes are developed through directed evolution, an iterative trial-and-error process that requires substantial time and experimental effort[1]. Computational enzyme design offers an alternative by predicting variants with desired properties. While thermodynamic properties such as stability can often be estimated using classical molecular mechanics (MM) simulations, catalytic activity remains considerably more challenging because it requires accurate evaluation of reaction mechanisms. Consequently, studies of enzyme activity typically rely on quantum mechanical (QM) or QM/MM methods, whose computational cost limits the number of variants that can be screened[2].

Here, we introduce a methodology based on non-equilibrium alchemical transformations to predict mutation-induced changes in activation free energies $\Delta\Delta G^{\ddagger}$. Because the approach employs a purely classical molecular description, it is at least an order of magnitude faster than conventional QM/MM calculations. To obtain bonded parameters, we developed a new scheme combining the inversed Hessian matrix of the transition state and the modified Seminario method [3]. Nonbonded parameters are derived from substrate electron densities using the atoms-in-molecules method [4]. The proposed approach is tested in two enzymatic systems: Crotonyl-CoA Carboxylase/Reductase and Dihydrofolate Reductase. The results show that the alchemical transformations successfully reproduce both experimental values and trends, with errors close to the chemical precision (1 kcal/mol)[5]. Finally, we applied our workflow to an Old Yellow Enzyme variant that catalyzes C–C bond formation via an aldol reaction. The method identified a novel double mutant (Y187F/T130A) with a twofold increase in activity relative to the native enzyme. Experimental validation showed good agreement with the computational predictions, demonstrating the accuracy of the workflow and its potential for high-throughput enzyme engineering.



$$\Delta\Delta G^{\ddagger} = \Delta G^{\ddagger}_{mut} - \Delta G^{\ddagger}_{wt} = \Delta G^{Alch}_{TS} - \Delta G^{Alch}_{RS}$$

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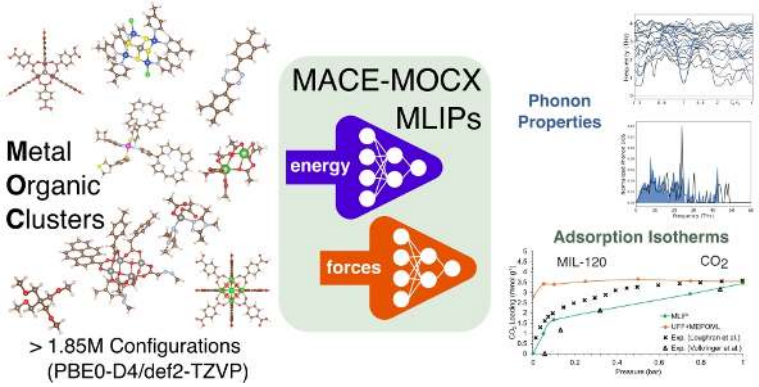
O37

Greater than the sum of its parts—Efficient ML Interatomic Potentials for DFT-Quality Simulations of MOFs via Fragment-Based Approaches.

Marco Gibaldi and Tom K. Woo

Department of Chemistry and Biomolecular Sciences, University of Ottawa

Computational materials discovery must often compromise accuracy to accommodate the massive quantity of calculations necessary. Pioneering studies in foundation or "universal" machine-learned interatomic potentials (MLIPs), such as MACE-MP0 and OMol25, provide avenues towards performing simulations with near quantum mechanical accuracy at more feasible costs. Until now, efforts have largely focused on molecular or inorganic structures and limited developments exist for periodic crystal systems such as metal-organic frameworks (MOFs). Realizing a generalizable MOF-based MLIP is challenging due to the breadth of chemical substructures that must be considered to fully encompass this diverse structure class. This work pursues this universal model objective by training on 1.85M density functional theory (DFT) configurations (PBE0-D4/def2-TZVP) sampled from ca. 1.4k MOF-derived structural building units (SBUs). These MLIPs were applied directly in the calculation of relevant vibrational properties and achieved commensurate performance—>20% RMSE improvements in phonon-derived thermal properties (i.e. entropy, free energy, and heat capacity) and total DOS/band frequencies—with more specialized potentials developed on smaller collections (i.e. hundreds) of crystal structures (e.g., MACE-MP-MOFs-v2). Additionally, their usage as foundation models for fine-tuning protocols which target DFT-quality guest adsorption simulations was probed using adsorbate-loaded configurations. CO_2 and H_2O adsorption isotherms generated in this manner showed excellent agreement with experimental data even in cases with prior documented issues caused by classical force field-based parameters (e.g., group 13 elements, low pressure, etc.). These findings highlight the promise of applying lower-cost data generation on diverse molecular fragment libraries towards MLIP-accelerated studies of related periodic crystal structures.



O38

Surrogate Reliability and Applicability Domain in ML-Driven CO_2 Adsorption Screening of Metal–Organic Frameworks

Kimia Shahbazi and Mark Thachuk

Department of Chemistry, University of British Columbia

Machine learning surrogates enable rapid screening of metal–organic frameworks (MOFs) for CO2 capture, yet their reliability on candidates outside the training distribution remains poorly characterized. We train Tabular Transformer regressors on 324,107 ToBaCCo-generated hypothetical MOFs to predict CO2 uptake and heat of adsorption at P = 0.15 bar and T = 298 K. Each MOF is described by 15 mixed descriptors: geometric properties from Zeo++ (accessible surface area, pore volume, void fraction, pore diameters, channel/pocket counts) and categorical identifiers (metal node, organic linker, topology). The uptake model achieves R2 = 0.8765 ± 0.0026 (RMSE = 0.1872 ± 0.0019 mmol/g) by 5-fold stratified cross-validation, outperforming linear regression, random forest, XGBoost, MLP, and CatBoost baselines. SHAP feature attribution reveals a physically interpretable relationship between pore geometry and predicted uptake: MOFs with narrow micropores (low void fraction) adsorb more CO2 per gram than those with large, open pores. This reflects confinement-dominated adsorption at low partial pressure, where gas molecules interact with multiple pore walls simultaneously, producing stronger binding than in wide pores far from saturation. Linker identity modulates this effect, producing substantial variation at equivalent void fractions — indicating that linker chemistry is a major design lever alongside pore geometry. We deploy the surrogate on 34 generated candidates and validate against RASPA2 Grand Canonical Monte Carlo (GCMC) at 298 K, revealing two independent failure modes. First, 76% of candidates lie outside the training distribution by Mahalanobis distance (a measure of how far descriptor values fall from the training population). Error severity depends on topology: well-represented topologies (nbo, sra) show modest errors (0.25 mmol/g), while under-represented topologies (bcu) show much larger errors (1.27 mmol/g). Second, some statistically in-domain candidates still show large errors due to a descriptor–simulation mismatch. The Zeo++ analysis uses a hard-sphere probe to assess CO2 accessibility and reports zero accessible surface area and volume for these structures, indicating no CO2-accessible porosity. However, the GCMC force-field simulation finds that CO2 can energetically penetrate these borderline micropores, yielding non-zero adsorption. This mismatch is invisible to distribution-based screening and produces errors of 1.0–1.7 mmol/g. A key question is whether the surrogate can estimate its own uncertainty on novel candidates. We test this with conformal prediction, which constructs intervals calibrated to contain the true value 90% of the time. On held-out data these intervals achieve 90% coverage, but on generated candidates coverage collapses to 40%. Reweighting to correct for the distribution shift recovers coverage to 64% but falls short of the target, showing that post-hoc uncertainty estimates alone are insufficient. Two-stage prescreening — first verifying that Zeo++ reports meaningful CO2-accessible porosity,

then checking that the candidate lies within the training distribution — provides a more robust reliability guarantee. The only validated-reliable design rule is a Cu-paddlewheel pcu framework with ethynyl-type linkers, consistent with the confinement physics identified by SHAP.

O39

Symmetry-Protected Excitonic Quantum Batteries: From Optical Charging to Controlled Discharge

Gabriel Hanna

Department of Chemistry, University of Alberta

Quantum batteries are nanoscale systems that store and release energy by exploiting uniquely quantum mechanical features such as coherence, entanglement, and symmetry. In this presentation, I will give an overview of our group's work on excitonic quantum batteries, built from coupled quantum systems that store excitation energy in symmetry-protected dark states which do not emit light and are therefore long-lived. I will introduce the basic concepts using chemically intuitive ring and stacked-ring motifs, and show how a simple laser-charging protocol can funnel energy into dark states via nearby bright states. Using open quantum dynamics simulations, we demonstrate that these dark states can store energy, not just excited-state population, with minimal loss, and that energy can be released on demand by introducing controlled symmetry-breaking perturbations.

I will then discuss how battery geometry, coupling strengths, laser timing, and disorder (static defects, thermal motion, dephasing) affect charging, storage, and discharge, and identify design rules and operating windows that should be accessible in real systems such as molecular aggregates, excitonic materials, or designer nanostructures. Finally, I will highlight our recent work on tailoring the coupling between the battery and an energy sink to enhance exciton extraction rates, and on constructing chemically explicit exciton models parametrized from electronic structure calculations. Together, these studies provide practical design principles for experimentally testable excitonic quantum battery architectures.

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O40

Double-duty generative models of amorphous materials

Lena Simine

McGill University

Amorphous materials form a vast, yet vastly underutilized, class of materials. Computational simulations help in making some sense of their properties, but for the most part, the reach of computational methods remains limited. In the first part of the talk, I will explain how we use generative machine learning within the framework of the Morphological Autoregressive Protocol (MAP) to extend nanoscale samples into the mesoscale and to hunt for new physics in glassy systems. Two case studies that focus on amorphous graphene and on glass-forming liquids will be used to demonstrate MAP's double-duty utility: 1) as a sampling algorithm to obtain sufficiently large samples for property prediction, and 2) as a characterization tool, for example, to diagnose dynamic heterogeneity in fragile glasses.

O41

OPTIMIZING TRANSITION METAL-BASED MATERIALS FOR CO2 CAPTURE AND CONVERSION

Kulbir Ghuman, Lakshmi Anil, and Tanay Sahu

Institut National de la Recherche Scientifique

The functionality of the materials used for energy applications is critically determined by the physical properties of small active regions, such as dopants, dislocations, interfaces, grain boundaries, etc. The capability to manipulate and utilize the inevitable disorder in materials, whether due to the finite-dimensional defects (such as vacancies, dopants, grain boundaries) or due to the complete atomic randomness (as in amorphous materials), can bring innovation in designing energy materials. With the increase in computational material science capabilities, it is now possible to understand the complexity present in materials due to various defects, resulting in pathways required for optimizing their efficiencies. In this talk, I will present a critical overview of recent computational advances in the design of sustainable materials for light- and electric field-driven CO_2 capture, as well as for CO_2 conversion into fuels and value-added chemicals through photocatalysis. I'll provide a comprehensive review of our research efforts, which involve employing traditional methods like density functional theory (DFT), alongside leveraging the data they generate to implement machine learning techniques, thereby accelerating the discovery of transition metal-based materials for these vital applications.

O42

Computational Chemistry as a Tool for Targeted Radionuclide Therapy (TRT)

Cen Li[1], Yang Gao[2], and **Georg Schreckenbach**[1]

[1] *University of Manitoba*

[2] *University of Electronic Science and Technology of China*

Targeted radionuclide therapy (TRT), including targeted alpha therapy (TAT), is a relatively new and highly promising approach to cancer therapy. It relies on bifunctional chelators (BFC) that, on the one hand, specifically target the cancer tissue via covalent attachment to a disease targeting vector, and on the other hand strongly encapsulate the radionuclide (227-Th, 225-Ac, 197-Hg, 89-Zr, etc.). An ideal BFC should be highly selective for the radionuclide of interest. As a further extension, the therapeutic function (by way of the radionuclide) is extended by diagnostic imaging to achieve theranostics that enables real-time monitoring of the radiopharmaceutical agents.

Computational quantum chemistry has reached a point where it can make meaningful contributions to ligand design for TRT, by providing (i) background information and understanding of the fundamental chemistry of radioactive elements, (ii) computational characterization of existing ligands and radionuclide metal complexes, (iii) proposing novel designs for TRT and theranostic agents. In our experience, this works particularly well if done in close collaborations with the broader experimental efforts.

In this presentation, I will present examples from our work in this area, illustrating some of the challenges, the computational approaches taken, and the questions to be asked.

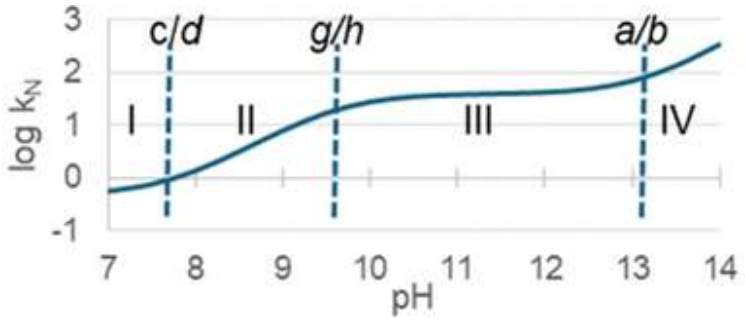
O43

Potential-of-Mean-Force vs Free-Energy Surfaces for pH-Dependent Mechanisms: The Case of Peptide Bond Formation in Ester Aminolysis

Allan East

University of Regina

A 2024 JACS paper presented a potential-of-mean-force (PMF) study that failed to locate the famed tetrahedral intermediate in the mechanism of aminolysis of esters (amine + ester → amide + alcohol), causing the authors to question the existence of the intermediate. The resolution of the problem is a fascinating foray into pH-dependent kinetics, the effect of pH on free-energy surfaces (FES) of reactions, and the delicate issue of presenting microsteps (e.g. proton-transfer) in chemical mechanisms. The talk will start with the 1968 Blackburn-Jencks mechanism and rate law, with a fresh presentation showing the four pH regions resulting from kinetics studies (the evidence for an intermediate). How this information should affect FES profiles (and the issue of microsteps) is then presented. Finally, the issues surrounding PMF representations of FES profiles are presented. Improved understanding of how PMF profiles relate to FES profiles will aid in the application of molecular dynamics simulation to mechanism elucidation.



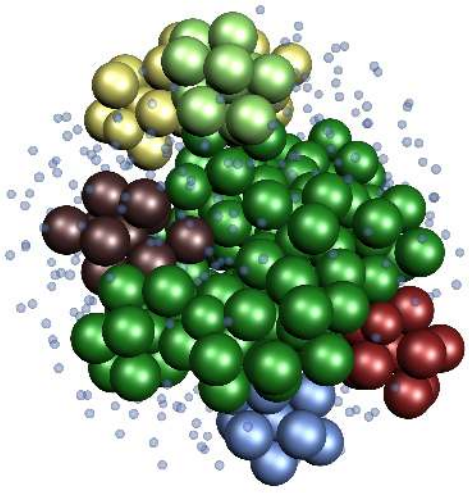
O44

Liquid nanodrolpets: From glass formation to liquid-liquid phase transitions.

Richard K Bowles

Department of Chemistry, University of Saskatchewan

Small aerosol droplets, ranging in size from 1-10 nm, play a central role in the chemistry and physics of the atmosphere. They affect climate by absorbing and reflecting solar radiation, enhance ice nucleation and act as solvent vessels, or heterogeneous surfaces, for important atmospheric chemical reactions. The physical state of the droplets influence all these processes, but nanoscale systems often exhibit unique phase behaviour and their properties become size dependent. This talk will discuss two nanoscale phase transitions. First, we will examine the nature of the glass transition in nanoparticle systems using molecular dynamics simulation, and compare their thermodynamic and dynamic behaviour with bulk glass forming systems. Second, we will develop a small systems liquid-drop model to describe how systems size effects liquid-liquid phase transitions, and examine how the presence of a liquid-liquid phase transition in the droplets influences condensation from the vapour.



II. Poster Presentations

P1

Path Integral Monte Carlo for Nanomolecular Assemblies of Water Molecules using Normal-Mode Sampling

Nithin Aaron[1] and Pierre-Nicholas Roy[2]

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Here, we develop the normal-mode sampling algorithm, an importance sampling method specifically designed for path-integral quantum Monte Carlo simulations of flexible molecular systems. This work is motivated by the desire to include vibrational degrees of freedom in numerical studies of confined molecular lattices.

We first introduce a novel density matrix factorization that arises from decomposing our system Hamiltonian into its harmonic and anharmonic terms. The normal-mode sampling algorithm is then constructed using this factorization.

Finally, we validate our normal-mode sampling algorithm in the context of path-integral quantum Monte Carlo simulations of several flexible molecular systems, namely the water monomer, dimer, and a few equilibrium geometries of the hexamer. For each of these systems, we calculate the ground-state energy and various structural properties, benchmarking our results against exact diagonalization, path integral molecular dynamics, and diffusion Monte Carlo studies from the literature.

We also propose applying this methodology to study quantum phase transitions in one-dimensional chains and higher-dimensional lattices of water molecules.

P2

Electron Correlation and Scalar Relativity in QTAIM

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The quantum theory of atoms in molecules (QTAIM) as originally formulated Prof. R.F.W. Bader and coworkers is a successful method for computing atomic properties within a nonrelativistic quantum mechanical framework.[1] Prof. R.F.W. Bader and coworkers showed that QTAIM satisfies the Schwinger principle of stationary action and as such justifying its utility for computing atomic properties in a nonrelativistic setting. [1, 2] Relativity is critical when computing properties of chemical systems that include nuclei with atomic number larger than 37.[3] It has been demonstrated how to formulate QTAIM to include relativistic effects in defining a proper quantum subsystem that satisfies Schwinger's principle of stationary action for the Scalar-Relativistic Zeroth-Order Regular Approximation (SR-ZORA) Hamiltonian.[4-6] Given that the concept of an atom in a molecule is satisfied even when relativistic corrections are included a more practical question remains: What level of theory is needed to obtain an accurate computation of a property? This of course means, what level of relativity, correlation method, and basis set is needed to for a reliable calculation of a property? In this presentation, the formulation of QTAIM from the Schwinger Principle at the nonrelativistic and SR-ZORA level of theory will be reviewed. Several properties at different levels of theory will be shown and provide intuition to properties that are sensitive to scalar-relativistic corrections, electron correlation, or both.[7]

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P3

Warning! The Negative Divergence of the Stress Tensor Will Not Always Yield the Ehrenfest Force

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The Ehrenfest force is the force an electron feels due to the external potential and the other electrons in the system.1,2 It can be computed as the property density of the negative gradient of the potential. This approach requires both the density and the pair-density. A convenient alternative way to compute the Ehrenfest force is by taking the negative divergence of the stress tensor.3-5 This approach relies only on the density matrix. However, other stress tensors can be formulated that can yield to the Ehrenfest force suggesting there is ambiguity in the stress tensor. In fact, there are many definitions of the stress tensors in the literature, particularly ones that depend on the density matrix and the density.2,5-8 It is shown here explicitly for the first time which of these stress tensors will yield the Ehrenfest force which will not yield the Ehrenfest force and how much the quantities generated differ.2,5

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P4

Gaussian process regression for ground and excited state dynamics

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Accurate trajectory surface hopping simulations are often limited by the high cost of electronic structure calculations, particularly when many trajectories are required to obtain statistically meaningful nonadiabatic dynamics. These simulations require smooth potential energy surfaces and nuclear gradients, which DFT/MRCI and other stochastic approaches cannot provide. Therefore, we develop Gaussian process regression (GPR) surrogate models for on-the-fly molecular dynamics, with the goal of enabling efficient nonadiabatic trajectory surface hopping on expensive electronic structure surfaces.

Initially, we apply the GPR framework to the simpler case of ground-state dynamics, before extending this approach to surface hopping. We utilise a Bayesian Committee Machine framework, which aggregates multiple independently trained GPR surrogates to enable efficient, highly accurate predictions. We test this approach on ground-state hydrogen peroxide dynamics, as well as excited-state surface hopping dynamics in ammonia using model potentials.

These results show that GPR-based surrogate models can reproduce key features of both ground state and nonadiabatic dynamics while substantially reducing the number of direct surface evaluations required. As well as providing a method to perform dynamics using electronic structure methods where gradients are unavailable or expensive, this approach produces a highly efficient trained potential energy surface for subsequent simulations and analysis.

P5

Mapping the Conformational Druggability of the Human Pocketome

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The identification of small molecules binding to biological targets is the central dogma of drug discovery, a challenging endeavour marked by a failure rate exceeding 90%. Structure-based virtual screening is a ligand discovery tool used to triage chemical libraries against the structure of a protein target at a much larger scale than wet-lab screens. Recent advances in chemoproteomics are rapidly mapping all the potential druggable sites encoded by the human genome, collectively known as the human pocketome. Concurrently, innovative approaches like ultra-large chemical libraries and artificial intelligence (AI) methods are paving the way for a new era in drug discovery. Yet only 3% of human proteins have been targeted with drug-like molecules to date. Indeed, emerging targets lacking known ligands remain very challenging for methods like docking and AI generative design, due to the arduous nature of identifying target conformations suitable for computational design when no confirmed ligands are known. To fill this gap, we seek to leverage machine learning (ML) to accurately predict druggable structures of binding sites from experimental or computational ensembles, without requiring prior knowledge of ligands nor human intervention. To this end, we first focus on developing a structural database of druggable conformations for known human protein targets, starting by developing compelling decoy molecule sets that closely simulate prospective library screens. The conformational druggabilities of the targets are then explored by combining biomolecular simulations and large-scale docking of active-decoy libraries. As such, the resulting database is a valuable resource for training ML models for forecasting structural druggability, thus guiding target selection for optimized computational ligand screening and design. Our work will open the door to the investigation of many new potential drug targets, including those modeled with Alpha Fold (AF) that represent an unprecedented, yet untapped resource in the field.

P6

Differentiable Optimization of Classical Force Fields for Quantum Dots

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Density Functional Theory (DFT) is currently the standard reference method for modeling Quantum Dots (QDs) and Nanocrystals (NCs). However, the high computational cost of Ab Initio Molecular Dynamics (AIMD) prohibits the study of long-timescale evolution in these systems. To bridge this gap, classical force fields and Machine Learning Interatomic Potentials (MLIPs) are often trained to reproduce DFT potential energy surfaces.

While MLIPs have achieved near-DFT accuracy, they present significant drawbacks. They act as uninterpretable "black boxes" that obscure physical insights, require vast amounts of training data, and often fail catastrophically in out-of-distribution (OOD) scenarios. Furthermore, MLIPs remain significantly more computationally expensive than classical potentials during production runs. Classical potentials offer a lighter alternative but face their own parameterization challenges. Current programs, particularly for QDs, rely on gradient-free stochastic search techniques, such as Genetic Algorithms or Monte Carlo methods, to fit parameters. These methods require expensive iterative simulations and frequently fail to converge on optimal parameters, especially within high-dimensional spaces or complex loss landscapes. Additionally, these programs are often biased toward bulk properties, neglecting the unique surface physics of finite nanostructures.

In this work, we present a differentiable parameterization framework designed to overcome these limitations. By reformulating the fitting process as a gradient-based optimization problem rather than a stochastic search, we eliminate the need for iterative simulations during training. Our approach utilizes automatic differentiation to match energies and forces against DFT data directly, enabling the rapid parameterization of finite nanostructures. This method reduces computational time from days to minutes while maintaining the physical rigor of classical potentials through physics-aware constraints.

P7

DeepAPD: Graph Neural Network Prediction of Adsorbate Binding Landscapes in Metal–Organic Frameworks

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Metal–organic frameworks (MOFs) are promising materials for gas storage and separation because their pore environments can be chemically tuned across a vast design space. However, identifying the local adsorption environments that control performance remains challenging. Adsorbate probability distributions (APDs), obtained from molecular simulation, provide a direct atomistic picture of where adsorbates reside within MOF pores, with local maxima corresponding to binding sites. Despite their value, converging APDs using grand canonical Monte Carlo (GCMC) simulations is computationally expensive and therefore difficult to deploy in high-throughput materials discovery.

In this work, we present DeepAPD, an equivariant graph neural network for rapid prediction of APDs in MOFs. The model represents the framework as a periodic atomistic graph and uses spatial probe nodes to infer adsorbate probability values at arbitrary positions in the unit cell, enabling resolution-independent prediction of three-dimensional APDs. As a proof of concept, DeepAPD was trained on GCMC-derived APDs for approximately 23,000 MOFs for methane at 1 and 65 bar and xenon at 1 bar. Novel binding site analysis/extraction algorithms are employed to assess the performance of DeepAPD. The resulting models reproduce simulated APDs with high similarity and reliably identify high occupancy binding sites (positional errors of 0.15 – 0.30 Å). DeepAPD also outperforms simple guest–host energy-grid approaches, particularly under conditions where guest–guest interactions play a significant role in the adsorption free-energy landscape.

By replacing expensive GCMC sampling with a reliable surrogate model, DeepAPD enables APDs and binding sites to be generated in seconds to minutes rather than hours to days. The advantage of DeepAPD is expected to become even more advantageous for more complex adsorbates (e.g., CO_2, H_2O), where conventional GCMC sampling becomes more computationally demanding. This work introduces a route to incorporating atomistically resolved adsorption information into high-throughput MOF screening, binding-site mining, and future generative design workflows for porous materials.

P8

First–Principles Prediction of Fundamental and Optical Gaps in Metal–Organic Frameworks

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Metal-organic frameworks (MOFs) are promising materials for light-driven applications. While their optical properties have been widely investigated experimentally, the relationship between optical absorption, charged excitations, and the underlying electronic structure remains difficult to assess computationally. In particular, most computational studies of MOF photophysics have compared ground-state DFT band gaps, often obtained using standard hybrid functionals such as PBE0 or HSE06, with experimental UV-vis absorption onsets. Although these methods can sometimes appear to reproduce experiment, such agreement is fortuitous since the quantities being compared are not equivalent. Experimental absorption onsets reflect neutral excitations and therefore include excitonic and vibrational effects, which are expected to be significant in MOFs. In contrast, the fundamental gap describes charged excitations and determines the thermodynamic driving force for charge separation. Distinguishing these quantities is essential for understanding whether photoexcitation in MOFs produces bound excitons or charge carriers that can participate in light-driven processes. The goal of this work is to clarify the relationship between ground-state electronic structure, optical absorption, and charge separation in MOFs by explicitly computing both charged and neutral excitations, along with the excitonic and vibrational effects that connect them to experiment.

Here, we calculate charged and neutral excitation energies in a representative set of ten widely studied MOFs. Fundamental gaps are computed using many-body perturbation theory within the G_0W_0 approximation and compared with non-empirically tuned range-separated hybrid functionals, including Wannier-localized optimally tuned screened range-separated hybrid (WOT-SRSH) and doubly screened hybrid (DSH) functionals. Optical gaps and absorption spectra were then obtained using the Bethe–Salpeter equation and time-dependent DFT using the DSH functional (TD-DSH), with zero-point and finite-temperature phonon renormalization incorporated through finite-difference electron–phonon coupling calculations.

WOT-SRSH and DSH reproduce G_0W_0@PBE fundamental gaps well, with mean absolute errors of 0.31 and 0.42 eV, respectively, and strong linear correlations across the MOF set. For neutral excitations, TD-DSH and G_0W_0@PBE-BSE optical gaps show improved agreement with experiment after phonon corrections, whereas conventional TD-PBE0 underestimates exciton binding energies. Across the MOF set, excitons are strongly bound, often exceeding 1 eV, demonstrating that optical and fundamental gaps must be treated as distinct quantities when evaluating MOFs for light-driven applications. These results establish practical computational routes for predicting charged and neutral excitations in MOFs and show that apparent agreement between hybrid DFT band gaps and absorption measurements can obscure the underlying excited-state physics.

P9

A First-Principles-Based Force Field for N-Heterocyclic Carbene Gold Nanoclusters

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Gold nanoclusters (GNCs) protected by N-heterocyclic carbenes (NHCs) and halides are promising candidates for cancer therapy. These systems feature a superatomic gold core with closed-shell electronic structure, while NHC ligands form a stabilizing shell that enhances photophysical properties[2]. Their chemical, physical, and biological behavior can be tuned through ligand modification. Molecular dynamics (MD) simulations are essential for describing their behavior in biological environments and predicting macroscopic properties such as stability and solubility, but their accuracy depends on the quality of the underlying force field. Recent force fields for NHC–GNCs provide reliable bonded parameters compatible with AMBER, but nonbonded interactions remain less developed[2]. Atomic charges are typically derived from RESP fitting, while van der Waals parameters are adjusted to reproduce macroscopic observables, which may be insufficient for organometallic systems. Here, we introduce nonbonded parameters derived directly from electron density partitioning of NHC–GNCs. We provide Lennard-Jones parameters and atomic charges for mono- and bidentate NHC–Au_{13} clusters using the theory of atom-in-molecules[3] (AIM). The resulting AIM-based parameters reproduce electrostatic, dispersion, and Pauli repulsion energies at near ab initio accuracy. Their transferability is assessed across chemical environments, and charge redistribution in the gold core and ligands is analyzed to quantify coordination effects. Validation against electrostatic potentials and energy decomposition analyses shows robust performance, with particular accuracy in describing $\pi - \pi$ interactions between ligands.

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P10

Understanding the Quasiphase Transition of the Water-filled Carbon Nanotube with Quantum Simulations

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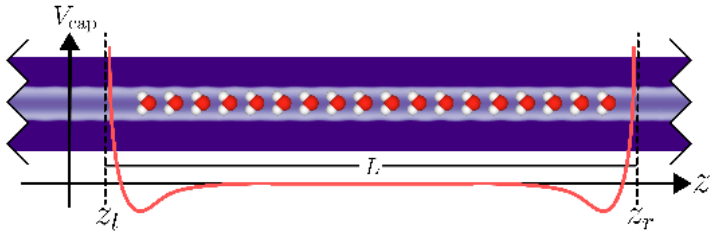
University of Waterloo

Confined water chains have been shown to display interesting properties, such as phase transitions (PTs), and these properties could be leveraged to create quantum devices. More specifically, a temperature-dependent quasi-PT was found experimentally for water-filled (6, 5) carbon nanotubes (CNT). Simulations have attempted to explain this PT, suggesting that it was caused by an orientational order to disorder transition in the dipoles of the water chain. However, this work was done with classical simulations, and presented only a limited analysis of the mechanisms at play. To address this and obtain a conclusive PT mechanism, we present our quantum simulations of this system where emphasis has been placed on creating realistic experimental conditions. Analytically-defined caps are used to investigate the system at the equilibrium density and precomputed discretized potential energies and forces help accelerate path integral molecular dynamics simulations to reach ergodicity. A wide range of temperatures are simulated to accurately capture the whole transition and the system size is changed to help pinpoint the PT's thermodynamic limit. The tools and methodology developed for the comprehensive study of the water-filled CNT will naturally lend themselves to other confined water systems, and studying these could enable tuning of the currently observed quantum properties or uncover new ones.



P11

Momentum-balance of atoms and molecules in ground and excited states

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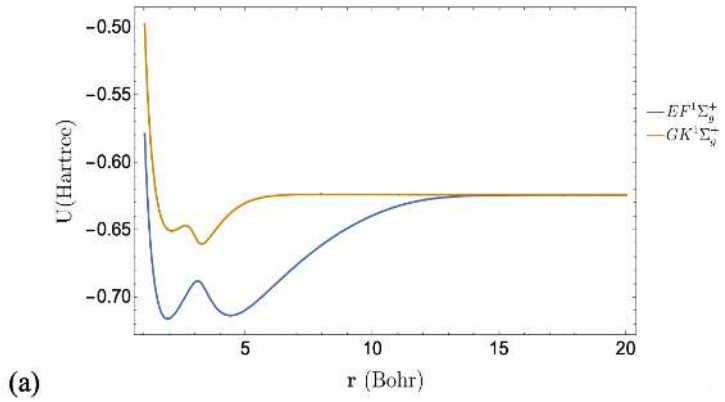
Our group has developed a quantitative tool called momentum balance, which uses two-electron density matrices, to understand correlated electron motion in ground and excited states (Todd & Hollett, 2021) of atoms and molecules. The momentum balance is a measure of correlated electron motion as the difference between probability that electrons have the same or opposite momentum. Highly accurate wavefunctions and their two-electron density matrices of varying spin multiplicity of atoms and molecules are calculated using the extrapolated Full Configuration Interaction approach within the Quantum Package 2.0 software. The two-electron density matrix is obtained from the wavefunctions and analyzed using in-house software, including calculating momentum balance, momentum balance density, and two-electron density. Our group has precisely obtained the correlated electron motion of the ground state of atoms using the proposed methods (Todd & Hollett, 2021). We also found impressive results for the excited states of H_2 molecule using the proposed methods. For instance, momentum balance can be used to describe the double wells in the potential energy curves of H_2 molecule (Figure 1) obtained at various electronic excited states (Wang et al, 2006; Nakashima & Nakatsuji, 2018). Momentum balance can also be used to assess how the relative spin (opposite or parallel) of electrons in atoms influences their relative motion, and how this motion changes in the excited states. This study will advance our understanding of correlated electron motion to develop better electronic structure models of the ground and excited states, efficient tools for chemistry and materials research.



(a)

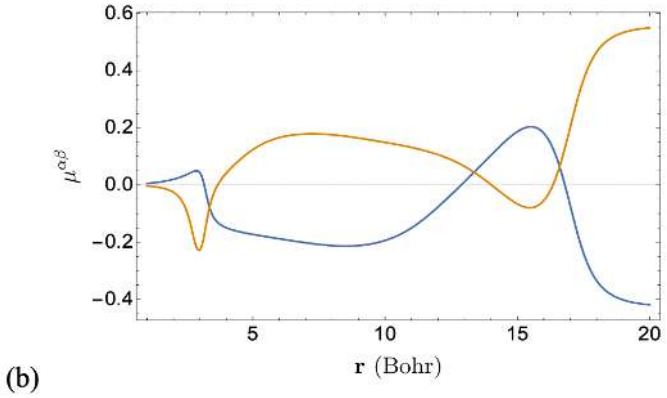


Figure 1: Potential energy (a) and momentum balance (b) curves of the excited states, $EF^1\Sigma_g^+$ and $GK^1\Sigma_g^+$, of H_2 molecule at varying internuclear distances. A change in momentum balance sign at the double wells of $EF^1\Sigma_g^+$ (1.90 Bohr & 4.40 Bohr) and $GK^1\Sigma_g^+$ (2.00 Bohr & 3.30 Bohr) excited states suggest a change in the relative motion of the electrons.

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P12

Constructing Atomic Multipole Moments Consistent with Electrostatic-Potential-Fitted Charges

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An accurate description of electrostatics is one of the crucial prerequisites for modeling chemical interactions and developing force fields. Molecular electrostatics can be represented by a multipole expansion of atom-centered moments; however, such atomic moments are not uniquely defined and depend on the underlying fitting or partitioning scheme. Fitting approaches are appealing because they reproduce the electrostatic potential directly, but they are often ill-conditioned and non-unique, making the resulting atomic moments sensitive to the fitting protocol and less transferable across chemical environments. Density-based partitioning offers an attractive alternative by deriving atomic moments directly from the molecular electron density, although existing methods vary in how accurately they reproduce electrostatics. Basis-space approaches such as Gaussian Distributed Multipole Analysis (GDMA) [1] are computationally efficient but can perform poorly at short range, whereas Hirshfeld-type methods are more robust and transferable, though still strongly dependent on the choice of proatom densities. Bridging the gap between fitting and partitioning approaches, we introduce a new method for constructing atomic densities consistent with charges fitted to the electrostatic potential (ESP), analogous to a recently proposed reverse-engineering approach for Charge Model 5.[2] Specifically, we use the charge-constrained Additive Variational Hirshfeld (c-AVH) framework[3] to obtain atomic densities consistent with ESP-fitted charges. This new approach, called ESP-c-AVH, is applied to diverse datasets of organic molecules, inorganic species, and protein fragments. We compare the multipole moments produced by ESP-c-AVH with those obtained from several other methods, including ESP-fitted dipoles and quadrupoles[4], GDMA, and Hirshfeld-based partitioning schemes like Minimal Basis Iterative Stockholder (MBIS)[5]. We assess and compare their performance to reproduce molecular multipole moments and electrostatic potential. The results show that ESP-c-AVH moments perform competitively with MBIS and, in most cases, outperform GDMA and ESP-fitted moments.

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P13

Computing vibrational spectra with collocation: using complicated kinetic energy operators and handling non-symmetry in large matrices

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Computing a vibrational spectrum numerically with a full-quantum treatment often involves expanding the unknown wavefunction as a linear combination of basis functions and solving the time-independent Schrödinger equation to obtain the expansion coefficients. This procedure yields a matrix eigenvalue problem that must be solved using linear algebra algorithms.

Collocation provides a formulation of the matrix eigenvalue problem by demanding that the Schrödinger equation be satisfied at collocation points in space. The collocation matrix eigenvalue problem is

$$\mathbf{B}^{-1}(\mathbf{T}+\mathbf{VB})\mathbf{U}=\mathbf{UE}$$

$$\mathbf{B}_{\alpha i}=b_i(\mathbf{q}_\alpha),\quad \mathbf{T}_{\alpha i}=Tb_i(\mathbf{q})\Big|_{\mathbf{q}=\mathbf{q}_\alpha},\quad \mathbf{V}_{\alpha\beta}=\delta_{\alpha\beta}V(\mathbf{q}_\alpha)\ .$$

$b_i(\mathbf{q})$ is a basis function, $\mathbf{q}_\alpha$ a collocation point, T is the kinetic energy operator, and $V(\mathbf{q})$ is the Born-Oppenheimer potential energy surface. The advantage of collocation over more common methods, such as variational methods, is greater flexibility. Collocation facilitates the use of optimized basis functions and coordinates. There is more leeway in the choice of points since no quadrature is needed.

In this work we show that collocation can be used with any choice of internal coordinates using a numerical kinetic energy operator, and can be combined with 1D contracted stretch, bend and torsion functions to efficiently compute the vibrational spectrum of flexible molecules.

The size of the basis set used can be large, thus iterative eigensolvers are preferred when computing a vibrational spectrum. They compute eigenvalues by means of matrix-vector products, they are more efficient than direct eigensolvers when only a portion of the spectrum is needed, and they avoid storing a prohibitively large matrix. Collocation yields non-symmetric matrices, and standard iterative methods for non-symmetric eigenvalue problems have unappealing computer memory requirements when a large number of eigenvalues is sought.

We present a new, low-storage iterative method based on the block Sakurai-Sugiura (SS) contour integration method to extract many eigenvalues from a single series of matrix-vector products. The method uses a multi-shift quasi-minimal residual (QMR) procedure to iteratively compute the quantities needed to use the SS method in any portion of the spectrum from a single series of matrix-vector products, enabling a systematic search of the eigenvalues.

P14

A machine learning model for determining bond types in metal-containing compounds

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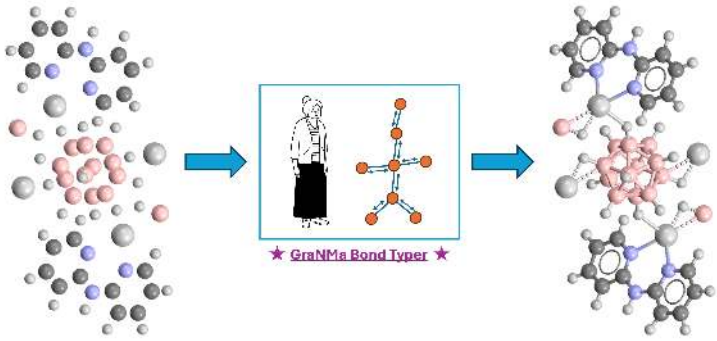
The covalent bond type (e.g. single, double, aromatic, delocalized, etc) is a fundamental chemical concept whose evaluation is necessary in a vast array of common applications, such as calculating formal charges or constructing arrow-pushing diagrams to describe chemical reactions. In the cheminformatics and machine learning spaces, they are commonly used as descriptors to encode molecular structure information. Although determining bond types in organic molecules is trivial, their evaluation in metal-containing periodic structures, given only the atomic coordinates, can be challenging. For this, the tools in the CSD Python API are widely used. However, this library is proprietary, requiring paid licensing to be used, and is known to produce poor and inconsistent results for organometallic compounds and metal-organic frameworks (MOFs).



We are developing an edge-centric message-passing graph neural network called GraNMa (GRAph Neural network MAchine learned) Bond Typer to compute the covalent bond types in molecular and periodic structures containing metal-ligand bonds, such as organometallic compounds and MOFs, using only the 3D atomic coordinates. Current efforts are directed towards refining the model and improving bond type assignment in cases where the CSD Python API is known to be incorrect, such as metal-coordinating heterocycles. Ultimately, this metal-aware machine learning approach will allow GraNMa Bond Typer to be an open-source replacement for the CSD Python API bond typer.

P15

Application of the DFT/MRCI Method to Spin-Orbit Coupling and L-edge X-ray Spectroscopy

Teagan Shane Costain[1], Alena Macdonald[1], Songhao Bao[1], Simon Neville[2], and Michael Schuurman[2]

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[2] *National Research Council*

L-edge core-level spectroscopy presents a significant challenge for electronic structure theory due to the simultaneous importance of electron correlation, orbital relaxation, and spin–orbit coupling effects. In this work, the density functional theory/multireference configuration interaction (DFT/MRCI) method is applied to the calculation of spin–orbit-coupled core-excited and core-ionized states relevant to L-edge X-ray absorption and X-ray photoelectron spectroscopy. The approach combines a density functional reference description with a multiconfigurational treatment of excited-state correlation, enabling computationally efficient treatment of electronically complex states while retaining important configuration interaction effects. Applications to heteroatom-containing molecular systems involving phosphorus, silicon, sulfur, and chlorine demonstrate that DFT/MRCI reproduces key spectral features, including spin–orbit splittings, state mixing, and relative transition intensities, at substantially lower computational cost than many conventional multireference approaches. These results highlight the potential of DFT/MRCI as a practical framework for the simulation of relativistic core-level spectroscopies in larger molecular systems.

P16

Investigating the effects of solvation on the thermodynamics of the ammonia oxidation reaction (AOR)

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The ammonia oxidation reaction (AOR) is an electrochemical reaction that produces hydrogen and nitrogen gas from ammonia. Due to the relevance of hydrogen gas in the implementation of green energy, optimizing the catalysis of this reaction is essential for the application of the AOR [1]. The density functional theory (DFT) models commonly used to study this reaction are often vacuum based, and can lack accuracy in comparison to solvated models [2]. This project will use an explicit solvent model to accurately represent the water-metal interaction, along with the computational hydrogen electrode to observe the effects of this reaction system on the thermodynamics of the AOR. The system will be modelled on iridium, platinum, palladium, and ruthenium surfaces, which allows for direct comparison to our previously published vacuum-only AOR study [3]. A number of different overlayer configurations and molecular orientations are investigated to ensure an accurate picture of the water-metal interaction is established. We investigate two different solvation models: one in which the water hexamer is kept intact with the adsorbate added in (the add. model), and one with the water hexamer interrupted by inserting the adsorbate into the hexamer, replacing one of the water molecules (the rep. model). Our results thus far indicate that the add. model tends to result in a water structure more displaced from the surface, whereas the rep. model experiences disruptions of the perfect hexagonal lattice to form new tessellation patterns. In addition, the water molecules arranged in a predominantly H-up pattern tends to increase the work function compared to a predominantly H-down pattern, consistent with previous studies [4]. The overall effect of solvation on the reaction pathway is a tendency to decrease the limiting potential for Pt and Ru. These results highlight the importance of incorporating solvent effects into DFT models of electrochemical reactions.

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P17

Machine learning for accelerating the calculation of dynamic correlation energies from a two-electron density functional

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A functional that accounts for the short-range dynamic correlation energy has been derived by our research group in terms of the two-electron density, rather than the usual one-electron density or the occasional on-top density found in [1]. The two-electron density functional (TDF) is based on modelling the correlated pair density under the constraints of an electron-electron cusp and evaluating its effects on the electron-electron potential energy. Employment of the aforementioned functional, however, becomes computationally expensive as electronic systems get larger and more complex. The present work focuses on accelerating the calculation of TDF dynamic correlation energies using a supervised machine learning approach. Accordingly, the accuracy of a multi-layer perceptron algorithm for predicting the desired energies will be examined once a full hyperparameter optimization is carried out.

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P18

Quantifying the impact of nuclear quantum effects on furanoside conformations

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Despite the ubiquity of carbohydrates, assessment of their conformations is challenging for experimental approaches alone. This is especially true for cyclic sugars with five-membered rings (known as furanosides) due to their high degree of flexibility.[1,2] To understand their structure, furanosides are studied with nuclear magnetic resonance (NMR) spectroscopy.[3,4] The structural information contained in vicinal proton-proton coupling constants ($^3J_{H,H}$) from NMR is deciphered through computational studies. Past theoretical work in this domain has relied on classical molecular dynamics to reconstruct detailed conformational distributions.[3–5] Classical molecular dynamics methods omit nuclear quantum effects, which are known to have a delocalizing effect on the positions and momenta of low-mass atoms like protons. Here, we investigate the impact of nuclear quantum effects on the conformational distributions of arabinofuranosides, along with the impact had on calculated $^3J_{H,H}$ values.

To quantify the impact of nuclear quantum effects on arabinofuranosides, this work uses path integral molecular dynamics simulations of arabinofuranoside monomers. The results from the path integral approach show the broadening of dihedral angle distributions within the monomers, with slight differences in the final $^3J_{H,H}$ values compared to classical simulation results. This work informs future analyses of flexible chemical structures that rely on proton positions as a primary source of conformational information. Additionally, it indicates whether the addition of nuclear quantum effects has broader consequences on structural properties. This can be considered in other biochemical simulations that are sensitive to conformational changes, such as in binding studies.[6]

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P19

Self-consistent correlation-factor generalized Kohn-Sham theory using automatic differentiation

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We present a self-consistent implementation of the correlation-factor model for exchange and correlation within the generalized Kohn–Sham (gKS) framework. In the correlation-factor approach, the exchange-correlation hole is written as the product of a model exchange hole and a correlation factor,

$$\rho_{xc}(\mathbf{r}, u) = f_c(\mathbf{r}, u)\rho_x(\mathbf{r}, u),$$

where $\mathbf{r}$ is the reference position and $u = |\mathbf{r}' - \mathbf{r}|$ is the electron–electron separation[1,2]. In the present implementation, the exchange hole is represented with a generalized Becke–Roussel form [2,3], and the resulting hole model is used to construct the exchange-correlation energy,

$$E_{xc} = \int d^3r\, \rho(\mathbf{r}) \int d^3u\, \frac{\rho_{xc}(\mathbf{r}, u)}{2u}.$$

A central difficulty in the self-consistent use of such functionals is that the energy depends explicitly on orbital quantities and nonstandard intermediate ingredients. Accordingly, the effective gKS contribution is obtained from derivatives with respect to the orbitals rather than from a purely multiplicative density derivative,

$$\hat{v}^{\mathrm{gKS}}_{xc,\sigma}\phi_{i\sigma}(\mathbf{r}) = \frac{\delta E_{xc}}{\delta \phi^*_{i\sigma}(\mathbf{r})}.$$

To evaluate these derivatives efficiently and robustly, we implement the functional in Python using JAX and employ automatic differentiation to generate the orbital-dependent terms entering the self-consistent-field cycle [4]. This avoids lengthy manual derivations and fragile finite-difference procedures.

The implementation is assessed through self-consistent calculations for representative atoms and molecules. The results show that automatic differentiation provides a practical and stable route to fully self-consistent gKS calculations with correlation-factor-based functionals. More generally, this work demonstrates that physically motivated, hole-based exchange-correlation models can be brought to the self-consistent level in a flexible computational framework suitable for further functional development.

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P20

Simulating the shape memory of polyurethanes by molecular dynamics

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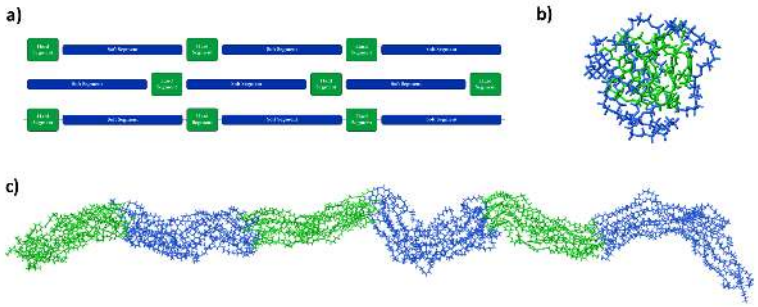
Shape memory is the unique property of polymer materials to recover their permanent shape after deformation. The most promising applications of such materials are found in medicine and aerospace [1]. To introduce this property to the material, the chemical structure should contain two different segments. Soft Segments ensure the flexibility of the polymer, allowing for the shape reorganization, while Hard Segments promote shape fixity by forming strong interchain interactions (Fig.1). The strength and character of interchain hydrogen bonds between Hard Segments have been elucidated in the previous research [2].



In this study, the shape memory property of polyurethane copolymers is investigated by means of molecular dynamics. Model systems are built based on the experimentally synthesized copolymers reported in the literature [3]. The shape memory cycle is simulated by changing temperature and pressure, to which model systems are exposed. The structure-property relationship is established based on the shape recovery ratios of copolymer models with different chemical compositions. Comparison to experimental data allows for verifying and aligning the results with the experimentally performed tests. The performed research is the foundation for further detailed multiscale investigation of shape memory copolymers morphology and physicochemical properties.

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P21

Achieving near chemical accuracy with atom-centered potential augmented M06-2X

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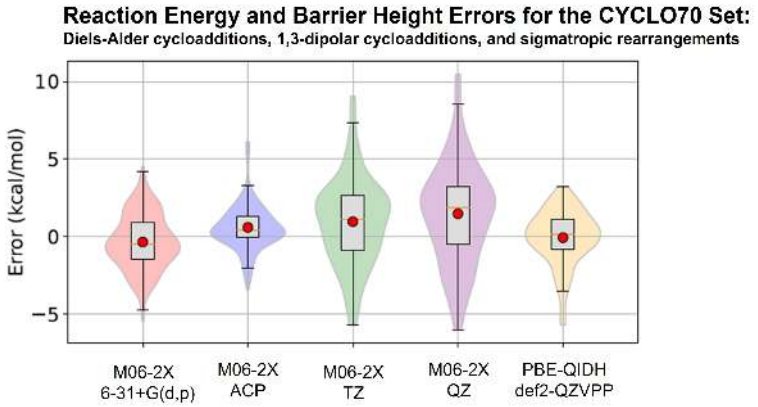
The calculation of accurate thermodynamic properties, such as activation and reaction free energies, is an essential tool for elucidating reaction mechanisms. The method most commonly employed, density functional theory (DFT), generally falls short of chemical accuracy (1 kcal/mol error), resulting in order-of-magnitude errors in the calculation of equilibrium constants and rate constants. The inaccuracy of common exchange-correlation functionals is compounded by the use of small and medium-sized basis sets, which are mandatory for molecular systems of realistic size. In previous works, we proposed energy corrections based atom-centered potentials (ACPs) to mitigate functional and basis set incompleteness error. ACPs are one-electron potentials that, when applied with a functional and basis set combination, yield results comparable to a higher level of theory with little or no additional computational cost.

In this work, we developed ACPs for thermochemical calculations using M06-2X/6-31+G(d,p). The resulting M06-2X/6-31+G(d,p)-ACP method is tested on a variety of cases, demonstrating excellent performance for thermochemistry and kinetics calculations well outside the parametrization set, particularly for reaction energies and barrier heights of moderately large system. At the same, time M06-2X/6-31+G(d,p)-ACP retains the low cost of the uncorrected functional and basis set combination.



P22

When the Environment Matters Most: Polarizable-Embedding QM/MM for Multi-Photon Absorption in Red Fluorescent Proteins

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Multi-photon absorption in fluorescent proteins (FPs) is highly sensitive to the surrounding protein environment, yet most computational studies treat the chromophore in isolation, which limits protein-specific non-linear response. This work presents a polarizable-embedding (PE), quantum mechanical/molecular mechanical (QM/MM), investigation of two- and three-photon absorption (2PA and 3PA) across seven red fluorescent proteins, including DsRed, mCherry, mPlum, mStrawberry, TagRFP, mRFP1, and mKate. The calculated 2PA cross sections ($\sigma^{2\mathrm{PA}}$) show strong agreement with experiment, reproducing both the overall magnitude and the relative ordering across the protein series. The proteins predicted to exhibit the largest $\sigma^{2\mathrm{PA}}$ values, DsRed, TagRFP, and mKate, match the experimental ranking, with maximum absolute deviations of 23 GM (DsRed) and 31 GM (TagRFP). For the remaining proteins, the deviations do not exceed 6 GM. Furthermore, the computed trends correlate with changes in permanent dipole moments ($|\Delta\mu|$), supporting the physical consistency of the PE description in capturing environment-driven charge redistribution. Absolute 3PA cross sections ($\sigma^{3\mathrm{PA}}$) are reported for all investigated FPs. Although direct quantitative comparison with experiment is limited to action cross sections, the predicted ordering for the available systems is consistent with reported measurements. Moreover, the computed 3PA trends closely follow those obtained for 2PA, preserving the same general ranking of non-linear response across the FPs. Overall, this work demonstrates that PE is essential for reproducing multi-photon absorption magnitudes in FPs and provides the first description of both 2PA and 3PA across multiple red fluorescent proteins.

P23

A First-Principles Reformulation of Reduced Density Matrix Functional Theory

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For several decades, density functional theory (DFT) has served as a cornerstone of electronic structure theory. Its exceptional combination of accuracy and computational efficiency has established it as the dominant method in chemistry, materials science, and condensed matter physics. Nevertheless, despite its widespread success, DFT exhibits important shortcomings, particularly for strongly correlated systems, where static and dynamic electron correlation are not treated on an equal footing.

Reduced density matrix functional theory (RDMFT) represents an appealing alternative by taking the one-body reduced density matrix, rather than the electronic density, as the fundamental variable. This more informative quantity naturally captures essential features of electronic correlation. However, RDMFT has traditionally lacked several of the key theoretical ingredients that underpin the success of Kohn–Sham DFT.

In this presentation, I will introduce a first-principles reformulation of RDMFT based on a fictitious partially interacting reference system, analogous to the Kohn–Sham framework. The corresponding effective Hamiltonian establishes a rigorous theoretical foundation and, importantly, allows for the construction of an adiabatic connection within RDMFT. We investigate the characteristics of this adiabatic connection and show how it can be employed both to study correlation effects and to inform the development of improved functionals.

By incorporating an adiabatic connection into RDMFT, we restore one of the most valuable conceptual frameworks in modern electronic structure theory within a density-matrix-based formalism. This development provides a systematic route for designing and assessing new functionals, bringing RDMFT substantially closer to becoming a practical and widely applicable alternative to conventional density functional theory.

P24

Implementation of Lattice-Mapped Coarse-Grained Equations of Motion for Simple Fluids

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Atomistic simulations become computationally expensive for large systems and long timescales, motivating the use of coarse-graining (CG) methods that reduce the number of degrees of freedom by grouping atoms into beads. This approach enables the efficient study of complex systems, particularly in biology. The challenge, however, is that once we simplify the system, we must still maintain the underlying physics by constructing accurate coarse-grained potentials.

Conventional CG methods use fixed particle groupings to define coarse-grained variables. Lynn and Thachuk[1] developed a position-dependent mapping in which particles dynamically contribute to CG variables based on their positions, allowing the representation of systems where particles undergo diffusion. Building on this framework, Luo and Thachuk[2] developed a lattice-based CG approach for fluids, in which a generalized quadratic potential with multivariate Gaussian statistics represents the interactions. In this formulation, the CG potential can be written as

$$V(\mathbf{x}) = \frac{kT}{2}(\mathbf{x} - \boldsymbol{\mu}_x)^T \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu}_x) \tag{1}$$

where $\mathbf{x} = (\mathbf{M}, \mathbf{W})^T$, $\boldsymbol{\mu}_x$ is its mean, and $\boldsymbol{\Sigma}$ is the covariance matrix.

Subsequent developments extended the framework by incorporating fuzzy switching functions, which allow for smooth transitions of particles between adjacent regions.[3] Additionally, they derived analytic expressions for CG potential parameters that can be directly derived from the fluid properties.[4]

In this work, we study the behavior of the CG equations of motion using the expressions developed by Luo and Thachuk. The system is represented by partitioning the cubic box into n subcells of edge length 2ℓ. A mapping was established between each CG subcell's three-dimensional coordinates and a one-dimensional index, and vice versa. To eliminate surface effects and better approximate bulk behavior, periodic boundary conditions were applied. This introduced an indexing challenge near the boundaries, where the separation between two cells is defined as the minimum distance, which may occur within the same image or across periodic images. Using these corrected displacements, cell-cell interactions are classified by relative spatial configuration into closest, $\sqrt{2}$, and $\sqrt{3}$ neighbors, corresponding respectively to pairs differing by $\pm 2\ell$ in one, two, or three Cartesian coordinates.

Using the lattice mapping framework, the elements of the Σ matrix are evaluated through correlations among the W variables, between W and M, and among the M elements, together with the mean $\langle M \rangle$. Each correlation function is decomposed into one-particle and two-particle contributions, which are evaluated separately and then summed to obtain the total correlation. Initial validation is performed for a single-component fluid, with extensions to mixtures left for future work.

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P25

Computational modelling of Rare Earth adsorption on Zr-based MOFs

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Rare Earths (REs) are critical materials, and within their production, the most challenging step is the separation from primary and secondary sources, as well as individual separations. Conventional liquid-liquid extraction methods require several cycles with large volumes of solvents because of the close chemical similarities shared between them. Metal-Organic Frameworks (MOFs) are attractive candidates for solid-liquid separation: adsorption of solvated Rare Earths onto the linkers of MOFs can provide a versatile and reusable separation strategy. This work presents insights into interactions between selected RE3+ cations and some de novo MOFs, highlighting relative binding stabilities of MOF-REs pairs for separations. De novo framework structures are built and relaxed on atomic positions and lattice parameters. Structural analysis is done with Voronoi cell decomposition via Zeo++ software. The equilibrated structures were used to construct cluster and periodic models to study REs binding. Relative adsorption energies are estimated with density functional theory (DFT) and semiempirical methods (GFN1-xTB), as implemented in Amsterdam Modeling Suite. Most frameworks exhibit channels ranging from 5 to 20 Å, suitable for the diffusion of solvated rare-earth ions. The modeling of REs–MOF interactions points to preferential binding as a function of linker chelating angle and ionic radius. Differences in relative binding energies rise to 10 kcal/mol with broader chelating angles favoring larger REs (La, Ce) and narrower chelating angles for smaller REs (Lu, Y, Sc). This work on REs adsorption on MOFs is valuable as it provides insights into the separation potential of MOFs. Development of greener REs separations is increasingly important to meet their growing demand. The goal of this work correlates with Sholl and Lively statement in ”Seven chemical separations to change the world”: “Producing rare earths economically is a problem of separations, not availability ”.

P26

Disambiguating the Kinetic Energy Density

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The local kinetic energy (kinetic energy density) is widely used to interpret chemical bonding, yet its definition is inherently ambiguous. In addition, finite basis sets introduce artifacts that alter its behavior relative to the complete-basis-set limit. We present a general framework that resolves these ambiguities and systematically removes basis-set artifacts, yielding a well-defined and physically consistent kinetic energy density.

P27

Entropy Sinks the Convex Hull in Sodiated Black Phosphorus

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The development of Na-ion batteries (NIBs) is one route to practical, utility-scale energy storage with improved scalability and energy security, relative to Li-ion batteries (LIBs), especially within Europe and Canada. However, the intercalation-based graphite negative electrodes that provide LIBs such exceptional lifetime are fundamentally incompatible with NIBs, because Na intercalation in graphite is endergonic. Black phosphorus is structurally analogous to graphite, but does electrochemically intercalate Na, making it a potential alternative. Insertion electrodes (of which intercalation electrodes are a subset) are known to have a significant entropy contribution due to the large number of possible geometric configurations. The purpose of this work is to evaluate the significance of configurational entropy for DFT energy calculations of sodiated black phosphorus (Na_xP) electrodes. For these calculations, B86bPBE-XDM(Z) is used to include accurate representation of the interactions between adjacent black phosphorus layers, as well as intercalated Na atoms. Temperature-dependent electrode potential experiments are used to measure the entropy during sodiation of Na_xP, for $x \leq 0.5$. The results show that including configurational entropy decreases the energy of some stoichiometries below what is expected for the convex hull based on a single Na configuration. The implications of this work suggest new computational approaches are needed for properly determining the true convex hull of insertion and intercalation electrodes, which make up the vast majority of battery electrode materials.

P28

Using Vibrational Perturbation Theory to Elucidate the Effects of Hydrogen-Bonding Environment in the OD Stretching Region of $[Py^+\text{-}(CH_2)_n\text{-}COOD]_2[NTf_2^-]$ (n=1-9) Ionic Liquids

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Second-order vibrational perturbation theory (VPT2) provides an effective tool for obtaining anharmonic corrections to harmonic frequencies and intensities. With VPT2, we gain insights into the vibrational motions that are responsible for the peaks observed in the experimental spectrum. This is especially valuable for systems that contain hydrogen bonds. In this work, we examine the vibrational spectra of the $[Py^+\text{-}(CH_2)_n\text{-}COOD]_2[NTf_2^-]$ (n=1-9) ternary complexes, which contain a double hydrogen bond between the carboxylic acid groups in the cations. At n=1 a single peak is present in the OD stretching region of the spectrum, while for larger alkyl chain lengths (n=2-9), there are three peaks present in this region. Using VPT2 based on electronic structure calculations performed at the B3LYP/6-31+G** level of theory/basis set, we explore the changes in the hydrogen-bonding environment with increasing alkyl chain length, and how these changes affect the calculated spectra. We also explore the effects of the choice of resonance space used in the VPT2 calculation on the calculated spectrum. We find that the inclusion of 2:1 Fermi resonances between the OD stretch and the overtone in the OD bend is essential for obtaining agreement between the calculated and measured spectrum. We also find that as the chain length increases the OD stretching frequency decreases until it is lower in energy than the overtone in the OD bend, reflecting the increased hydrogen bond strength with increasing alkyl chain length.

P29

Analytical ground-state nuclear gradients for pair-natural-orbital-based MP2 and CC2 methods using localized virtual molecular orbitals

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Accelerating the evaluation of analytical nuclear energy gradients in wavefunction-based quantum chemical methods and extending these approaches to large molecular systems remain challenging tasks. In this work, we developed analytical nuclear gradients for second-order Møller-Plesset perturbation theory (MP2) employing pair-natural orbitals (PNOs) derived from orthonormal localized virtual molecular orbitals (LVMOs). In contrast to projected atomic orbital (PAO)-based formulations, our approach introduces two key distinctions. First, constraints arising from the LVMO construction are incorporated into the Lagrangian, which necessitates solving an additional Z-vector equation, namely the coupled-perturbed virtual localization (CP-VL) equation. Second, due to the orthonormal nature of the LVMOs, the derivatives of the PNO coefficients with respect to both MO coefficients and nuclear coordinates vanish, which simplifies the formulation of analytical energy gradients. Additionally, we developed an automatic derivation program to alleviate the technical complexity associated with deriving gradient expressions within the PNO framework. We also briefly report an extension of this framework to analytical nuclear gradients for the CC2 method using PNOs based on LVMOs for ground states.

P30

Evaluating the Bethe-Salpeter Equation within the GW Approximation (GW/BSE) for Excitation Energies of BODIPYs and Aza-BODIPYs

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Boron-dipyrromethenes (BODIPYs) are a class of fluorescent molecules known for their highly tuneable optical properties and diverse array of applications, ranging from medical imaging to photovoltaics. Due to multireference behaviour, strong electron correlation, and double excitation character, excited states of these systems are characteristically difficult to model computationally, complicating the theoretical design of novel BODIPY derivatives. Time-dependent density functional theory (TD-DFT) is known to consistently overestimate BODIPY excitation energies, producing mean absolute error (MAE) values above 0.3 eV; recent work suggests spin-scaled double hybrids with long-range correction can bring the MAE below 0.1 eV, albeit at significant computational cost. To assess an alternative approach, we turn to the Bethe-Salpeter equation within the GW approximation (GW/BSE), which has recently been gaining traction for its ability to eliminate many common issues of TD-DFT (such as the self-interaction error, unequal treatment of local and charge-transfer excitations, and strong functional dependence) at an equivalent computational cost. Using experimental excitation energies for a set of 17 substituted BODIPYs and aza-BODIPYs, we present a comprehensive benchmark of the GW/BSE method. The assessment includes analysis of basis set convergence with the aug-cc-pVnZ (n = D, T, Q) basis set series, comparison of evGW and G_0W_0 schemes to evaluate the effect of self-consistency in the GW calculation, and evaluation of the impact of different DFT starting points (PBE, LC-ωPBE, and PBE0 with varying levels of exact exchange). Results demonstrate that GW/BSE produces MAE values under 0.2 eV while maintaining strong linear correlations, significantly outperforming TD-DFT and cementing GW/BSE as a valuable tool for the prediction of BODIPY excitation energies and design of future BODIPY derivatives.

P31

Interacting Quantum Atoms (IQA) Energy Decomposition from Variational Hirshfeld Partitioning Methods

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Interacting Quantum Atoms (IQA) energy decomposition analysis partitions the molecular energy into intra- and interatomic contributions, with physically meaningful components such as kinetic, electron–electron, electron–nucleus, and nucleus–nucleus terms [1]. In this work, we present a Python implementation and performance assessment of the IQA framework developed within the QC-Devs Software Consortium [2]. Our modular and flexible implementation can be combined with any atoms-in-molecules partitioning scheme. In particular, we couple IQA with variational Hirshfeld methods [3] and compare the results against Quantum Theory of Atoms in Molecules (QTAIM) [4] for a series of diatomic molecules. We show that the resulting energy components generally align with chemical expectations, with Hirshfeld-based IQA offering improvements over QTAIM in some cases.

Because IQA analysis is computationally demanding, we present several performance optimization strategies, including just-in-time compilation, multiprocessing, and vectorization, that significantly accelerate the calculations. This achieves speedups of up to two orders of magnitude compared to our baseline implementations. The resulting implementation is computationally efficient, flexible, and currently supports a wide variety of Hirshfeld-based partitioning schemes. Through the QC-Devs ecosystem, the IQA module interfaces seamlessly with other packages, enabling straightforward use with different wavefunction file formats. Moreover, its modular Python architecture allows additional partitioning schemes to be incorporated with minimal effort. To the best of our knowledge, this is the first IQA implementation to support multiple Hirshfeld-based partitioning methods within a module and an extensible framework.

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P32

Site-Selective Ligand Discovery for an Acetylcholine Receptor Using Multi-Objective Screening

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The human muscle-type nicotinic acetylcholine receptor (nAChR) is an important pharmacological target whose activation involves rapid transition through intermediate pre-open states. Recent structural studies reveal that its two agonist-binding sites undergo independent and asynchronous conformational changes, creating an opportunity to identify ligands that preferentially engage one site over the other. Here, we applied a fragment-based screening workflow that combines a multi-objective machine-learning model with active learning to prioritize compounds from a fragment database. The model evaluates several binding-related features simultaneously and uses each screening round to guide the selection of new candidates. This approach enriched the candidate pool for fragments predicted to favor site-specific binding, and may provide a route toward ligands that probe, and potentially modulate, the asynchronous activation mechanism of the receptor.

P33

A Quantum Dynamics Study of cis- and trans-Stilbenes

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[2] *National Research Council Canada*

cis- and trans-Stilbene have a long-studied photochemistry arising from their photo-initiated isomerization process, in which the large-amplitude relative motion of the phenyl rings has led to the molecule being identified as a molecular switch. A quantitative description of the corresponding absorption spectrum would therefore be essential for a complete account of the ensuing dynamics. However, previous assignments of the absorption spectra for these molecules, which neglected the vibronic coupling effects, fail to properly characterize the spectra. We present here detailed analyses of the vibronic spectra of cis- and trans-stilbenes simulated from wavepacket propagation calculations using the multi-configuration time-dependent Hartree (MCTDH) method. To do so, vibronic coupling Hamiltonian models are constructed by direct fitting to diabatic potential matrices computed using the novel QD-DFT/MRCI(2) approach. Our simulated spectra reproduce the main features of the experimental spectra in solution. The role of intensity borrowing from transitions to ππ* states, and the excited state dynamics of each molecules, are also examined in our study.

P34

On the Equivalence of Two-Point Basis-Set Extrapolations and Robust Parameterization for Coupled Cluster and Double-Hybrid DFT Methods

Mark Iron

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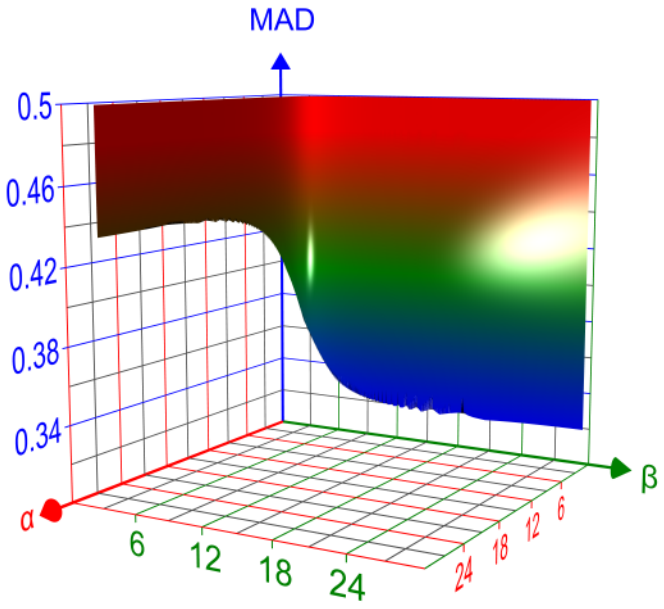
Basis set extrapolations are the foundation of many accurate thermochemical composite methods, allowing for much better accuracy at a much more favourable computational cost. Often, the extrapolation parameters are taken from the study by Neese and Valeev,[1] and these parameters are often used with other methods, such as MP2 or double-hybrid DFT. Because I was irked by some related issues, I decided to look carefully at a few issues related to basis extrapolations: (i) Is Neese and Valeev's stated method of simultaneously optimizing Hartree–Fock and CCSD(T) correlation energies justified; (ii) is it reasonable to optimize a single parameter for the CCSD(T) correlation energy; (iii) are the CCSD(T)-optimized parameters transferable to other methods, in particular double-hybrid DFT functionals; (iv) if the commonly used extrapolation methods (exponential–square root, exponential, power) for two basis sets can be reduced to a Schwenke-type form,[2–3] is there any meaning to the different methods; (v) is there any benefit to expanding their fitting set to include second-row elements? In this talk, I will present my results that I are currently under consideration for publication.



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P35

Effects of confinement on highly forbidden ortho-H2O to para-H2O isomerization

Justin Laroche[1], Thomas Putaud[1], Pierre-Nicolas Roy[2], and Patrick Ayotte[1]

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[2] *University of Waterloo*

Despite being forbidden by quantum mechanics, the isomerization reaction of the nuclear spin isomers (NSI) of the water molecule (ortho- H2O and para-H2O) is known to proceed readily under the confinement of inert matrices and endofullerenes1,2. The mechanism is thought to proceed through intra- and intermolecular hyperfine interactions, notably the nuclear spin-rotation and nuclear spin-spin couplings. Differences between interconversion kinetics reported for the various confinement media, as well as comparisons between calculated rates for the free H2O molecule in the gas-phase and under confinement can help understand the isotope and temperature dependence observed experimentally3. A simple confined rotor model is used to describe confinement effects on the ro-translational eigenstates while the quantum relaxation model is used to describe the interconversion rates between the NSI of water. Advances towards a quantitative description of confinement effects on the mechanism and rates for interconversion between the NSI of H2O will be examined in detail.

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P36

Direct dynamics simulation of photochemistry without the Born-Oppenheimer approximation

Edith Leal-Sánchez, Jong-Kwon Ha, and Ryan J. MacDonell

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The simulation of photochemical reactions requires a quantum mechanical treatment of electronic and nuclear dynamics. Most simulation approaches use the Born-Oppenheimer approximation and calculations of nonadiabatic couplings to evolve a wavefunction on a set of adiabatic electronic states. However, the use of adiabatic states present several challenges such as discontinuous surfaces, singular terms in the Hamiltonian, and double-valued boundary conditions. We present a direct dynamics approach for molecular vibronic dynamics which does not invoke the Born-Oppenheimer approximation simply by avoiding diagonalization of the electronic part of the Hamiltonian. Our approach evolves trajectories on linear combinations of configuration state function (CSF) surfaces, for which all terms in the Hamiltonian can be calculated exactly in a basis of active orbitals. By employing a diabatic propagation scheme for the orbitals, we ensure that all electronic terms vary smoothly as a function of nuclear coordinates. Using coupled-trajectory Ehrenfest dynamics, we avoid problems with basis-set completeness and decoherence while maintaining tractability for realistic molecules. We test our approach for LiH. In contrast with adiabatic electronic surfaces, we find that all CSF surfaces and couplings are smooth and integrable in the vicinity of avoided crossings. Comparisons of dynamics simulations with our approach and with adiabatic direct dynamics reveal the compromises in adiabatic approximations. Our approach performs highly accurate direct dynamics simulations at a comparable cost to conventional adiabatic-based techniques. It has the potential for further improvement with the adaptation of other electronic structure and vibronic dynamics methods.

P37

Exploring the non-linearity of linear free energy relationships and using machine learning to predict substituent effects

Shane Leonard and Robert Mawhinney

Lakehead University

Exploring the non-linearity of linear free energy relationships and using machine learning to predict substituent effects The Hammett equation has been a method widely used to analyze linear free energy relationships and the effects substituents produce for a molecule. Through computational analysis using 4 different backbones with 119 substituents discrepancies have been observed that are not easily explained by the original concept of the substituent and reaction constants relating to the molecular energy. When the only property changed is the substituent the energies should exhibit a 1 to 1 relationship regardless of backbone. Instead, non-insignificant variations are observed when comparing the reaction energy, Gibbs free energy and enthalpies. Previous studies1,2 investigating substituent properties and their effects on reaction energies found a strong relationship between the reaction energy and the x-component of the dipole moment attained from the analysis of the electron density. In this work, these relationships were greatly diminished when using a larger set of substituents (119). Machine learning methods were utilized, using 56 substituent property features. Linear regression, random forest, and symbolic regression models were examine. Best results were seen using symbolic regression generating the equation

$$-0.02481276\, e^{\left(-\frac{2}{(\alpha_{zz}^{\rho})^2 (H_c)^2 (\mu_x^c)^2\, e^{\left(j - 0.581364556795853 \frac{\mu_y^c}{DI(R,H)^2 + \alpha_{zx}^c} - \frac{\mu_y^c}{\lambda_{3,c}}\right)}}\right)}$$

$$j = -0.581364556795858 \frac{Q_{yz}(R)}{\alpha_{zx}^{\rho}} - 0.581364556795858\, Q_{zz} \lambda_{2,c}$$

Which generated r2 values of 0.8200 for Bicyclo pentane, 0.7223 for bicyclo octane and, 0.7379 for bicyclo undecane, as well as 0.7389, 0.7008 and 0.7076 for the three adamantane orientations used.

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P38

DFT Investigation of Ammonia Oxidation on CeO2 (100), (110), (111) Surfaces

Henry Lim, Brendan Paget, and Leanne Chen

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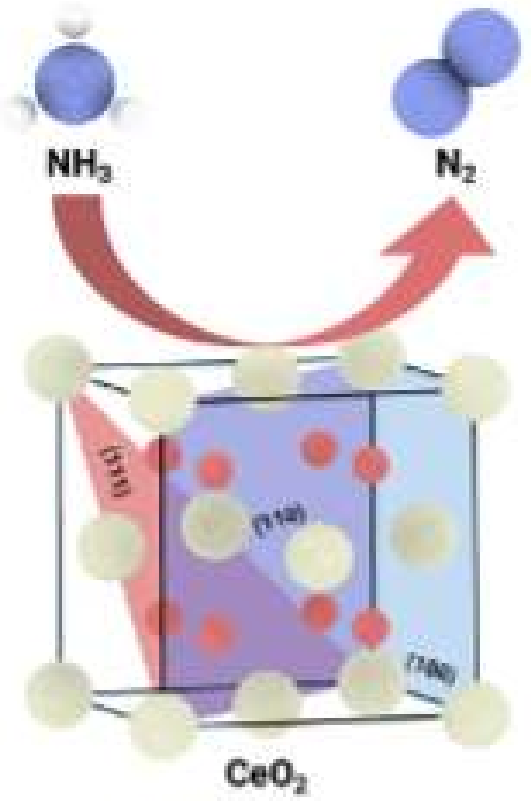
A key challenge preventing the widespread deployment of direct ammonia fuel cells (DAFCs) is the lack of inexpensive, active, and poison-resistant anode catalysts capable of efficiently carrying out the ammonia oxidation reaction (AOR). While transition-metal catalysts such as Pt exhibit good activity, their susceptibility to *N poisoning and high cost significantly limit their feasibility. Ceria (CeO2) has shown potential in related electrocatalytic reactions due to facet-dependent reducibility, oxygen vacancy formation, and tunable surface electronic structure. However, a comprehensive mechanistic understanding of AOR on ceria surfaces is lacking. Thus, this work outlines a density functional theory (DFT) investigation of AOR across the low-index ceria facets (111), (110), and (100) to identify the most active and selective surface for ammonia electrooxidation. Preliminary calculations reveal that the AOR intermediates were 0.3 eV more stable when accounting for spin-polarization relative to non-spin-polarized, demonstrating the significant role magnetic moments play for AOR on low-index ceria surfaces. Additionally, ceria (100) is predicted to be the most active surface due to having the greatest surface energy compared to ceria (110) and ceria (111); however, further calculations are required to confirm this trend for AOR.


NH3
N2
(111)
(110)
(100)
CeO2

P39

Feature Selection and Physics-Constrained Deep Neural Networks for the Representation of Exchange–Correlation Functionals

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This work presents a machine learning framework for representing exchange–correlation functionals within Density Functional Theory (DFT) [1]. Building on previous approaches in machine learning for exchange–correlation modeling [2,3,4], we introduce a reduced set of physically relevant descriptors to improve interpretability, reduce redundancy, and increase robustness. In addition, the Perdew–Burke–Ernzerhof (PBE) functional [5] is incorporated as a physical constraint to guide the training of deep neural networks and stabilize the optimization process. This physics-informed strategy enables the model to preserve known theoretical behaviors while learning complex data-driven corrections beyond conventional approximations. The combination of dimensionality reduction and embedded physical priors significantly improves training efficiency and mitigates overfitting. Furthermore, it enhances generalization across molecular systems and ensures greater numerical stability during self-consistent field calculations. Results demonstrate improved accuracy in predicting exchange–correlation energies compared to baseline approaches and show conceptual similarities with recent machine learning adaptations of hybrid functionals [6], while relying on a fundamentally different methodology. This work highlights the critical role of combining feature selection and physically grounded constraints for developing reliable and transferable machine learning models in constructing and representing exchange–correlation functionals.

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P40

MOF-HydrA: A lightweight and robust machine learning model for reconstructing missing protons in crystal structures of metal-organic frameworks

Jun Luo, Marco Gibaldi, and Tom Woo

University of Ottawa

Experimental 3D crystal structures are often missing proton positions due to the low electron density of hydrogen atoms. The positions of missing protons can be easily determined for typical organic molecules with heuristic algorithms; however, no robust methods exist for reconstructing missing protons near metal centers in organometallic compounds or crystalline solids such as metal-organic frameworks (MOFs). This is problematic when preparing structures for atomistic simulations since missing protons would lead to incorrect total charge or metal oxidation states of the compounds. Recent studies on structure errors of common MOF databases indicated that missing protons is a common error category. This work presents MOF-HydrA (HYDRrogen Assigner), a machine learning (ML) model based on the graph attention network that simultaneously predicts the number of missing protons for each atomic sites via ordinal classification and reconstructs the positions of the missing protons via edge regression coupled with post hoc trilateration. Most proton assignment tools can restore protons on organic linkers and terminal ligands but often fail to recognize missing protons near metal centers, particularly in bridging sites (e.g., μ-OH and μ-OH_2), whereas MOF-HydrA aims to restore missing protons for all atoms including the bridging sites between metal centers. Preliminary results achieved >99% accuracy for identifying the correct number of missing protons on each atomic site; and the model was capable of fully restoring all missing protons for >96% of MOF structures, with an average RMSD of <0.2 Å vs reference proton coordinates determined from DFT geometry optimization. When tested on structures with missing protons only on metal bridging sites, the model performed better reaching an accuracy of >98%. Currently, the model is still under active development to improve proton position precisions without relying on compute-intensive architectures (e.g., diffusion or large language models) or post hoc force field optimizations. Moreover, our proton assignment workflow offers flexible routines, such as fully autonomous restoration (replying solely on model predictions) or restoration on request (add designated number of protons based on a provided empirical formula).

P41

Quantum Criticality in Isotopically Substituted Dipolar Molecular Chains

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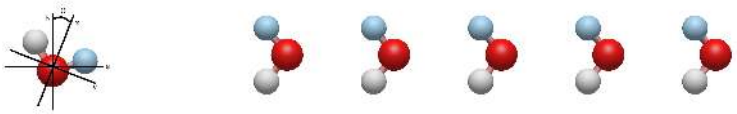
Quantum criticality in interacting systems of confined dipolar rotors is significant for the study of ground state quantum phenomena. This work aims to investigate the quantum critical behaviour of linear chains of small dipolar molecules, expanding on published results for the case of ordinary water (H_2O) and heavy water (D_2O). This will be achieved by studying how molecular isotopes, such as singly deuterated water (HDO), impact properties such as quantum entanglement, quantum phase transitions, and the excitation spectrum of the system. HDO breaks the particle exchange symmetry present in normal and heavy water, eliminating the restriction to either para- or ortho-water energy states. This project is computational in nature and, as such, requires the development of a mathematical model that describes the kinetic and potential energies for a system of rotating dipolar molecules. Due to its asymmetric mass distribution, the first steps will be to determine the principal axes of rotation and an appropriate basis for HDO. Then, a computational technique known as the Density Matrix Renormalization Group (DMRG) and the iTensor Julia library will be used to calculate the properties of interest, which will then be used to analyze the ground-state phase diagram of HDO. This work will provide a greater depth of knowledge regarding the conditions for quantum criticality in dipolar molecular chains and determine the effect of isotopically substituted asymmetric rotating molecules in these systems. The results of this work will identify potential selection criteria for additional molecular species of interest as candidates for applications in quantum devices or quantum computing as quantum bit (qubit) candidates.



P42

State-specific rate coefficients for H_2(v,j)+ H_2(v',j')

Margot Mandy

University of Northern British Columbia

The behaviour of molecular clouds in the interstellar medium is governed, in part, by the collisions of H_2 molecules. These provide ways of cooling interstellar shock fronts which can set the stage for star formation. The first mechanism has to do with collisional dissociation of molecular hydrogen. Since the probability of recombination of the molecule is negligible due to the low density regime, the dissociation energy is permanently removed from the shock. The second mechanism is due to the quadrupole emission from a collisionally excited molecule of a photon that has little chance of being reabsorbed. Depending on the density, this quadrupole emission can compete with the collisional processes. Because the gas is not in equilibrium, state-specific information is required for energy transfer and dissociation. With 348 (v,j) states for each molecule, this presents a computational challenge.

Current work is focused on dissociation. With calculations of over 800 combinations of initial states, preparations are being made to apply machine learning techniques to evaluate the over 60000 state-specific rate coefficients needed.

P43

General Optimizer (GOpt) with emphasis on transition state finding.

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We present a new molecular geometry optimization package which is especially robust for transition-state optimization. Key innovations include a new gradient-based trust-radius update, a robust way to define dihedral angles that avoids problems with near-linear bond angles, a way to selectively enhance the accuracy of the Hessian for key internal coordinates, and a robust way to select internal updates and update the Hessian expressed therein. By prioritizing software modularity, it became easy to support new features, allowing the Geometry Optimizer package to evolve into a General Optimizer. Gopt now supports an arbitrary number of coordinate transformations (allowing problems to be expressed in the coordinates for which the optimization/constraints are most efficiently expressed), myriad quasi-Newton methods, and alternative convergence criteria. This allows us, for example, to use Gopt in wavefunction optimization applications. In preparation for As Gopt 's imminent release, this talk will discuss key scientific innovations and software architecture decisions, while providing examples of use cases, especially those where Gopt is preferable to competing software.

P44

Tuning the Bath: How Spectral Density Parameters Control Exciton Discharge in an Open Quantum Battery

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Quantum batteries are quantum devices that exploit superposition, non-classical correlations, and entanglement to enhance energy charging and discharging. First proposed in 2013 [1], they have since inspired a wide range of theoretical models, yet experimental realizations remain limited, making accurate simulations essential for guiding device architectures and material choices. Here, we study exciton discharge dynamics in a symmetry-protected excitonic quantum battery [2,3], where an exciton is stored in a dark state that is shielded from loss channels by symmetry, and controlled symmetry breaking provides a tunable discharge mechanism (Figure 1).

To realistically capture the dynamics of such devices, we employ an open quantum systems framework, in which noise and dissipation from the environment are encoded via a spectral density. The environment is modeled as a collection of harmonic oscillators, and the spectral density specifies the frequency-dependent system-bath coupling, enabling energy relaxation, decoherence, and non-Markovian memory effects to be included without explicitly resolving all environmental degrees of freedom. We systematically investigate how the form of the spectral density influences the discharge dynamics, comparing Debye-Drude and Ohmic-like environments characterized by the Ohmicity exponent (s =0.5, 1.0, 1.5, and 3.0 correspond to sub-Ohmic, Ohmic, moderately super-Ohmic, and strongly super-Ohmic baths, respectively). We further examine the effects of the system-bath coupling strength and bath cutoff frequency. Across all parameter regimes studied, the Debye-Drude spectral density yields the largest exciton population transfer to the discharge site. For the Ohmic-like environments, the relative performance depends on both coupling strength and cutoff frequency. Increasing the coupling strength generally enhances population transfer for the Ohmic and moderately super-Ohmic baths, while the strongly super-Ohmic bath remains the least effective. In contrast, the sub-Ohmic bath exhibits a non-monotonic response, showing reduced transfer at stronger coupling. Variations in the cutoff frequency produce a different ordering of bath performance, indicating that the characteristic frequency distribution of the environment plays a distinct role from the overall coupling strength in determining discharge efficiency. These results clarify how environmental structure governs exciton transfer in a symmetry-protected quantum battery and help inform the design of physically realistic environments in experimentally realizable devices.

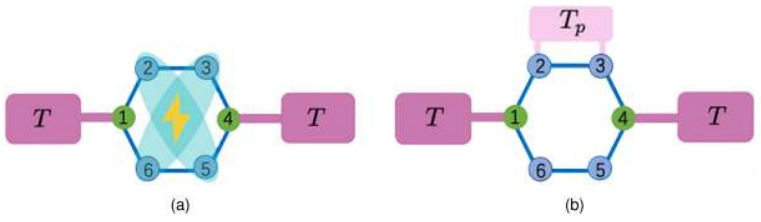

Figure 1: Architecture of the symmetry-protected excitonic quantum battery during the (a) storage phase and (b) discharge phase.

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P45

Machine Learning-Guided Identification of Allosteric Drug Binding Poses from Molecular Dynamics Simulations

Jacob Mastrandrea[1] and Mikko Karttunen[2,3]

[1] *Department of Chemistry, Western University, ON, Canada*

[2] *European Laboratory for Learning and Intelligent Systems (ELLIS) Institute Finland*

[3] *Department of Technical Physics, University of Eastern Finland*

Eumelanin is a heterogeneous, disordered biopolymer whose structural complexity complicates the identification of ligand binding sites, particularly allosteric interactions [1]. Diverse local environments and the absence of well-defined structure hinder atomistic characterization of binding mechanisms. We frame allosteric drug binding as a high-dimensional structural problem and introduce a computational pipeline for resolving binding modes from molecular simulation data. Molecular dynamics (MD) simulations generate trajectories of carbonic anhydrase inhibitors interacting with model eumelanin aggregates; these compounds [2] are experimentally classified as strong or weak binders, providing a ground truth for analysis. To extract structure from high-dimensional MD trajectories, we apply a feature representation based on a mixed radial–angular three-particle correlation function encoding local geometric and orientational relationships [3] between ligands and eumelanin subunits. This embedding is analyzed using unsupervised machine learning — t-SNE for dimensionality reduction and HDBSCAN for clustering — enabling identification of metastable binding states without prior labelling. The pipeline resolves distinct binding modes and identifies reproducible interaction motifs across independent simulations. The resulting embeddings capture physically interpretable features of ligand–eumelanin interactions and separate binding regimes, highlighting the value of combining representation learning with physics-based simulation to characterize allosteric binding in heterogeneous systems.

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P46

Active Learning for the Accelerated Design of Visible-Light Organic Photocatalysts

Andrea Minutti-Simoni and Rebecca Davis

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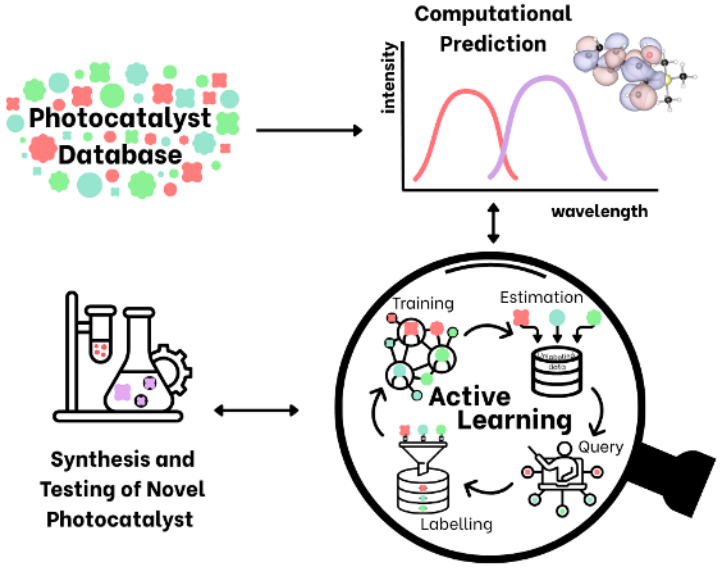
The accurate prediction of excited-state properties remains a key challenge in organic photocatalyst design, where experimental screening is often time- and resource-intensive. Computational methods, particularly time-dependent density functional theory (TD-DFT), offer a promising route to estimate photophysical descriptors, such as excited-state energies, absorption, and emission spectra, relevant to photocatalytic processes prior to synthesis, thereby enabling the prioritization of candidate molecules with optimized excited-state characteristics. In this work, a computational workflow is developed to support the efficient exploration of photocatalyst chemical space by combining quantum-chemical calculations with data-driven strategies. TD-DFT calculations using a range of hybrid and range-separated functionals in combination with multiple basis sets were evaluated against experimental values from the Joung et al. chromophore database to identify reliable approaches for predicting key photophysical observables. To ensure systematic coverage of chemical space, molecules were selected using cluster analysis, thereby identifying representative scaffolds while reducing computational cost. This workflow is designed to be integrated into an active learning algorithm, where iterative selection of informative candidates enables data-efficient and targeted exploration of chemical space, accelerating the discovery of organic photocatalysts with desired performance. By prioritizing the most promising candidates, this approach provides a rational basis for subsequent experimental validation and synthesis, bridging computational predictions with the development of new photocatalytic systems.



P47

Can Qubit Encodings Benefit Classical Simulations of Quantum Rotor Lattices?

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Computationally studying complex many-body phenomena such as quantum criticality is a difficult problem due to the exponential scaling of Hilbert space dimension with system sizes, and diverging correlation lengths at quantum critical points. One promising approach towards this involves adiabatically simulating the ground state of a qubit-encoded representation of the system in question, using a quantum device. To this end, many qubit encodings have been developed to map electronic and nuclear structure problems to spin-1/2 Hamiltonians. However, quantum hardware limitations currently prevent us from simulating sufficiently large lattices to probe macroscopic phenomena in many cases. In this work, we examine whether qubit encodings could be beneficial for classical simulations of many-body systems. We focus on quantum rotor lattices which can be used to model several exotic phenomena such as the formation of ferro-electric order in lattices of nano-confined dipolar molecules. Here, we first develop a qubit mapping for a d-dimensional dipolar planar rotor lattice and show that the resulting spin-1/2 Hamiltonian corresponds to a (d+1)-dimensional XXZ model, which is highly amenable to Stochastic Series Expansion Quantum Monte Carlo (SSE-QMC) approaches. SSE-QMC, in the past, has enjoyed remarkable success towards simulating critical phenomena in Bose-Hubbard and Ising models. Since SSE-QMC is unique to spin lattices, developing such algorithms for rotors directly is typically difficult. Using this XXZ representation, we develop an SSE algorithm for the qubit-mapped dipolar rotor lattice. Finally, we study the effectiveness of this approach by simulating the ground state of the dipolar planar rotor chain.

P48

Time-Dependent Coupled Cluster for Eigenstate Discovery: From One-Body Models Toward General Quantum Systems

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We present a unified framework for extracting eigenstate and thermal properties from time-dependent quantum dynamics, using coupled cluster and thermofield theory methods. This approach enables direct retrieval of eigenvalues and reduced density matrices. We apply this technique to a 1-body electronic Hamiltonian and further demonstrate the retrieval of thermal properties for diverse Hamiltonian systems including electronic, vibrational, and rotational models demonstrating exact access to thermal quantities across particle statistics.

P49

Data-Driven Framework for Rational Design of Gold Nanoclusters (AuNC)

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Gold nanoclusters (AuNCs), especially those stabilized by N-heterocyclic carbenes (NHC), are stable metal-based compounds that have attracted significant attention due to their tunable photophysical properties and potential applications in targeted cancer therapeutics. One of the main challenges in using NHC-stabilized AuNCs for light-mediated cancer therapy is the limited penetration of light through biological tissues due to scattering and absorption. As a result, identifying compounds with favorable photophysical properties in the near-infrared (NIR) region is a key challenge, as NIR light exhibits deeper tissue penetration and reduced scattering. Hence, researchers generally seek to develop compounds with maximized emission wavelengths. However, the exploration and optimization of NHC ligands through traditional experimental and computational methods can be both time-consuming and resource-intensive. To overcome these challenges, this project aims to develop a data-driven framework for chemical property prediction and accelerated discovery of NHC-AuNCs. We have created a dataset of more than 2500 NHC ligands and fragments derived from literature and synthesized compounds. These structures are then converted into Self- Referencing Embedded Strings (SELFIES), a robust molecular representation that guarantees the generation of chemically valid molecules by enforcing valence constraints. SELFIES are superior to the typically used Simplified Molecular Input Line Entry System (SMILES) representations, because not all of the SMILES strings correspond to a chemically valid structure. We use SELFIES as input to train a variational autoencoder (VAE), which learns a continuous latent representation of the ligand structures. During training, the molecular representations are compressed into low-dimensional latent vectors that capture the underlying structural features of the ligands. We then combine the learned latent space representations with the Bayesian optimization to identify ligands predicted to exhibit the highest emission wavelengths. This strategy allows us to leverage existing experimental and computational data to efficiently navigate the chemical space and identify promising candidate ligands for further experimental investigations.

P50

Near-Nuclear Quality Indicators for Gaussian-Type Wavefunctions

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Gaussian-type orbitals lack the electron–nucleus cusp, yet with appropriate construction they can still accurately capture the directional dependence of electron density in the near-nuclear region. This electron–nucleus anisotropy is reflected in the shape of cuspless electron densities and in the associated kinetic energy densities. We introduce simple anisotropy parameters and demonstrate that they provide sensitive and practical indicators of wavefunction quality in core regions.

P51

Einstein-Debye Model for Density-Functional Prediction of Vibrational Free Energies of Molecular Crystals

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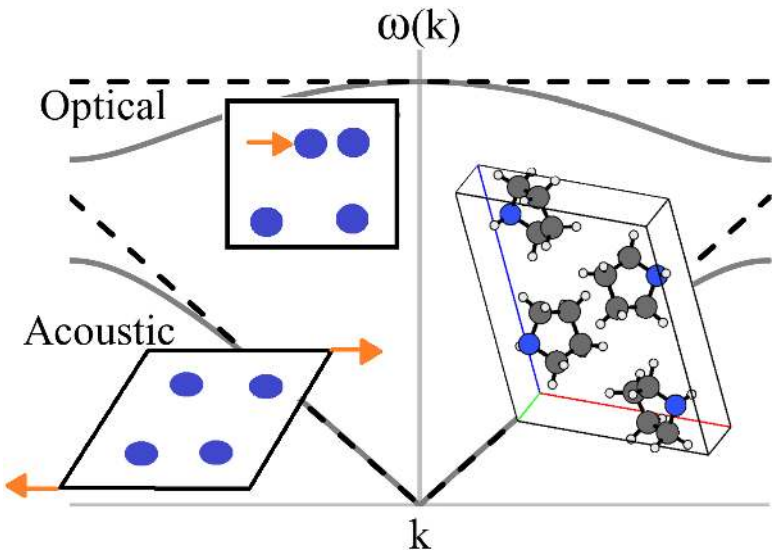
Accurately predicting the relative free energies of polymorphic molecular crystals is an important aspect of crystal structure prediction (CSP), which has found considerable utility in solid-form pharmaceutical development to assess the risk of conversion to a more stable, late-appearing polymorph. In this work, we investigated the Einstein-Debye phonon approximation to evaluate the vibrational free energy, F_{vib}, in conjunction with dispersion-corrected density-functional theory. Three data sets were considered: (1) The ”PV17’” benchmark of seventeen polymorph pairs exhibiting little or no conformational flexibility; (2) four large, flexible compounds that appeared in previous CSP blind tests; and (3) a new ”FP10” set of 10 highly flexible drug molecules that each have two or more known polymorphs. It was found that the Einstein-Debye approximation provides a good balance of accuracy and efficiency, giving mean absolute errors of ≤ 1.4 kJ/mol relative to full supercell calculations of F_{vib}, with a computational cost that is up to 4.5 times lower. Considering the magnitudes of free-energy differences between polymorphs, $|\Delta F_{\text{vib}}|$, a very broad distribution was observed, with average values in excess of 3 kJ/mol. In CSP studies of drug-like molecules, we recommend that ΔF_{vib} be considered for all candidate structures within at least ca. 6 kJ/mol of the global electronic-energy minimum to provide a high probability of identifying the correct free-energy minimum.



P52

Do Erroneous Metal-Organic Frameworks Impact the Predictive Abilities of Machine Learning Models for Different Gas Isotherms?

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Metal-organic frameworks (MOFs) have consistently attracted the attention of material scientists due to their diverse and tunable pore properties, which have made them viable candidates for many industrial chemical processes. To accelerate the identification and development of high-performing MOFs, "computationally ready" databases containing experimental and computer-generated structures have been curated, providing the raw data for high-throughput and machine-learning (ML) driven studies. Most of these studies have focused on screening or predicting various gas adsorption properties. Recent analysis found that CoRE-2019, the most-cited MOF database, has a structural error rate of 50%[1]. In other words, about half of the structures contain some sort of structural error, such as missing atoms and metal centres with impossible oxidation states. Unfortunately, hundreds of computational MOF studies have used this database "as is" to build and deploy machine learning models. The goal of this work was to assess how machine learning models trained and validated on "good" and "bad" structures would predict the adsorption properties of CO_2, Xe, H_2, and CH_4. To do so, six supervised regression models were trained, validated and tested on datasets consisting exclusively of chemically valid ("good") or chemically invalid MOFs ("bad"), or a 50:50 mix of these two types of structures ("mixed"). A reduction of up to 15% in the Pearson Correlation Coefficient (PCC) was observed when comparing the performance of models trained and tested on "mixed" datasets with those trained and tested exclusively on "good" sets. This effect was most pronounced for models predicting H_2 selectivity and CO_2 uptake, with an average reduction of of PCC=0.07 to PCC=0.08. The loss was least stark for models predicting Xe uptake and CH_4 working capacity, with the decline in accuracy amounting to only 0.4% and 0.3%, respectively. To this effect, it was noted that the performance of models trained on "mixed" sets could be improved by up to 7% if they were tested on sets of "good" structures instead of "mixed" ones. Nonetheless, this improvement depended heavily on the target. To summarize, chemically invalid metal-organic frameworks can negatively impact the performance of ML models. In fact, a noticeable decline in performance is observed when training and testing on "mixed" datasets relative to "good" datasets. This means that the hundreds of previous studies that utilized the CoRE-2019 database could be underreporting the accuracy for "good" top performers and structures.

[1]White, A. J. et al. High Structural Error Rates in "Computation-Ready" MOF Databases Discovered by Checking Metal Oxidation States. J. Am. Chem. Soc. 2025, 147 (21), 17579–17583. https://doi.org/10.1021/jacs.5c04914

P53

Determinant (Ratio) Methods: Efficient Computational Methods for Strongly Correlated Systems

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The full configuration interaction (FCI) method produces the most accurate results possible using a given basis set. Unfortunately, FCI is so computationally expensive that it can only be used on very small molecules. Popular methods including Hartree-Fock, tensor product state methods, and coupled cluster methods can be thought of as truncations or parameterizations of FCI that reduce the computational cost at the expense of accuracy, with different methods being more accurate for different types of systems.

We have developed a new type of method: the determinant ratio method. As the name suggests, the determinant ratio method parameterizes the FCI coefficients as products/ratios of several determinants. The method theoretically works well even with a small number of determinants, which should lead to good results using a much smaller number of parameters compared to similar tensor-product or exponential based methods. Since it does not truncate FCI and therefore includes contributions from all possible electron configurations, the method is suitable for studying strongly correlated systems. We have completed some preliminary testing of the method on a sequence of geometries representing the dissociation of BeH_2.

P54

Unraveling the Hidden Radical Character from Non-Radical Species

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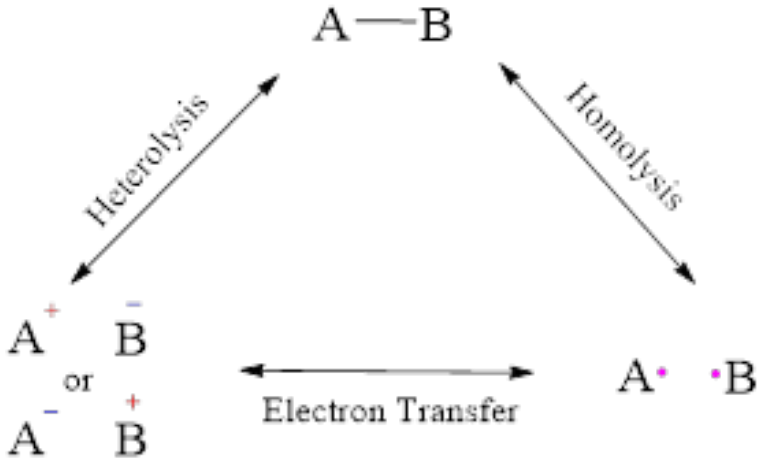
Hidden diradical character plays a critical yet often underappreciated role in controlling chemical reactivity and reaction mechanisms. Although any covalent bond may, in principle, access diradical configurations through homolysis, quantitative assessments of diradical character are highly method dependent and frequently difficult to interpret. To address this challenge, this work develops an integrated framework that combines valence bond (VB) theory, molecular orbital theory, and density functional theory, leveraging their complementary strengths to achieve a unified description of diradicaloid reactivity. This approach is first applied to para- and ortho-quinodimethane (p-QDM and o-QDM), which exhibit similar (30%) diradical character by VB analysis but markedly different reactivity. p-QDM dimerizes through an open-shell singlet (OSS) transition state, whereas o-QDM predominantly follows a concerted [4+2] cycloaddition, with radical pathways accessible only at elevated temperatures. These mechanistic distinctions are validated by high-level multireference calculations and supported experimentally by TEMPO addition studies, revealing unexpected radical-like reactivity. The framework is then extended to topochemical polymerization of para-aza-quinodimethane and to acid-catalyzed self-initiation of vinyl monomers, where electrostatic fields lower initiation temperatures to 70 °C, offering a greener alternative to conventional initiators. Finally, a novel trisulfide metathesis mechanism involving an OSS diradical transition state is identified, demonstrating the broad relevance of hidden diradical character beyond conjugated hydrocarbons. Overall, this work establishes hidden diradical character as a general and chemically consequential phenomenon, providing new opportunities for reaction design, polymer synthesis, and materials discovery.



P55

Comparative analysis of molecular conformer contributions to the Localization–Delocalization matrix and associated metrics

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we quantify electronic similarity across conformers of eight sulfur-containing systems using localization–delocalization matrices (LDMs) from Quantum Theory of Atoms in Molecule (QTAIM) and the Frobenius distance (FD) as a matrix-based metric. After conformer sampling and ωB97X-D/6-311G(2d, p) optimization, we analyzed 630 unique conformers (allyl mercaptan, 2-propenesulfenic acid, diallyl monosulfide, diallyl disulfide, diallyl trisulfide, allicin, and the E/Z isomers of ajoene). Conformers were grouped according to their QTAIM molecular graph classification into acyclic, ring critical point (RCP), or cage critical point (CCP) types. Pairwise FD-R values within and across topological classes are generally small (typically ≤ 0.10–0.15), indicating that electron density is largely preserved despite substantial conformational flexibility and distinct topological features, including ring and cage critical points. Analysis of bond critical points associ-ated with these features reveals low electron density and negligible delocalization, consistent with weak intramolecular interactions that modify topology without inducing significant electronic redistribution. Boltzmann-weighted averaging at 298 K yields ensemble-averaged LDMs that closely resemble those of the lowest-energy conformers, and equivalent trends are obtained at physiological temperature (≈ 300 K), confirming the robustness of the electronic similarity under thermally accessible conditions. A gradual increase in mean FD-R from R1 (≈ 0.07) to R4 (≈ 0.11) reflects modest electronic reorganization with increasing regime index rather than abrupt changes. Overall, these results demonstrate that pronounced topological differences do not necessarily imply significant electronic reorganization and establish LDM-based descriptors (FD, FD-W, N-loc, and N-deloc) as compact and robust measures of conformer similarity, clarifying when single-conformer approximations are adequate and providing a foundation for future extensions to protein-binding relevant conformational landscapes.

P56

Title: Allicin versus Allicin-Derived Sulfur Compounds: A Bond-Type-Specific Benchmarking Strategy for Antioxidant Studies

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Allicin, the principal organosulfur compound in garlic, has long been associated with a wide range of biological activities. However, emerging evidence suggests that these effects may arise not from allicin itself, but from sulfur compounds formed along its transformation pathways. To support this question computationally, we considered allicin together with a set of related sulfur compounds spanning its chemical transformation landscape, while accounting for the conformational space of each system, resulting in approximately 1100 structures overall. Because antioxidant activity is closely related to bond dissociation enthalpy (BDE), identifying a reliable model chemistry is a necessary first step. This is particularly challenging for sulfur-containing systems, as sulfur is highly polarizable, adopts multiple oxidation states, and participates in chemically distinct bonds such as S–S, S–O, C–S, S–H, C–H, and C–S=O. To address this complexity, a bond-type-specific benchmarking strategy was applied using a reference library of 77 representative organosulfur compounds [1]. Ten candidate model chemistries were assessed. Previous studies on sulfur-rich systems have identified hybrid functionals such as M06-2X and ωB97X-D as suitable for mechanistic thermochemistry and bond dissociation analysis [2,3]. Calculated and experimental BDEs were compared using mean absolute deviation, standard deviation, slope, intercept, skewness, and correlation coefficient. The mean absolute deviations remain largely within 4–7 kcal mol^{-1} across the tested model chemistries, indicating overall agreement with experimental sulfur-centered bond energetics. Among the tested methods, ωB97X-D/6-311G(2d,p) provided the best balance of accuracy, error symmetry, and computational efficiency, offering a practical framework for subsequent mechanistic and thermochemical evaluation of allicin and allicin-derived sulfur compounds.

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P57

Beyond the Ideal Lattice: A Hierarchical Fragment Approach to Engineering Defect Landscapes in 2D Materials

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While crystal engineering traditionally focuses on the rational design of the perfect periodic lattice, the functional properties of many next generation materials are governed fundamentally by their imperfections. Predicting the energetics of these dilute defects remains a challenge, as the large supercells required to minimize periodic image interactions are often computationally prohibitive. Here we introduce a solid state 'Amons' (Atom-in-Molecule) ansatz that bridges local chemical environments with bulk properties. Drawing on the supramolecular synthon concept where local motifs dictate global packing, we define 'solid state Amons' as a hierarchy of small, tractable periodic fragments that capture the essential local chemistry of the defect.

Using Density Functional Theory with the Exchange hole Dipole Moment (XDM) dispersion model to capture critical non covalent interactions, we analyze the finite size scaling of these fragments. This allows us to accurately extrapolate dilute limit energetics without requiring massive supercells. We validate the approach on substitutional defects and vacancies in h BN and graphene. Our results demonstrate that the defect landscape can be mapped with high fidelity at a fraction of the typical computational cost, providing a scalable tool for the inverse design of defect engineered materials.

P58

A Multifaceted Analysis of Angular and Radial Quadratures

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Numerical integration (quadrature) is essential for modern quantum-chemical calculations, especially density-functional theory methods and their post-processing (into atomic charges, bond orders, etc.). Many different integration methods for evaluating molecular properties have been proposed, but the most efficient seems to be the (generalized) Becke integration scheme, where each molecular property is broken into atomic contributions, which are integrated by combining a radial quadrature with an angular/spherical quadrature. We perform a series of comparative studies analyzing available one-dimensional quadratures, accompanying radial transforms, and angular quadratures reported in the literature. Specifically, we investigate how accurate these methods are for approximating integrals associated with the number of electrons, Kohn-Sham kinetic energy, and the dipole and quadrupole moments. In addition, to assess how well the grids compute numerical derivatives, we investigate the Weizsäcker kinetic energy.

P59

Evaluating Solvation Models for Theoretical Determination of Metal-Ligand Stability Constants

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The accurate determination of stability constants for metal-ligand complexes is central to understanding metal speciation in aqueous environments, yet it remains a significant challenge for theoretical modelling. Density-functional theory (DFT) calculations often struggle to produce reliable results for these species due to the complexities of modelling the solvation of charged metal complexes. In this work, we compare a purely implicit solvation model with a hybrid implicit/explicit approach to calculate the solvation energies of a series of metal cations, as well as the stability constants of their corresponding metal-cyanide and metal-glycinate complexes. By employing thermodynamic cycles to incorporate discrete water molecules into the first coordination sphere, we achieve a more physically realistic description of short-range solute-solvent interactions. While purely implicit models produce significant errors in solvation energies, the hybrid approach substantially improves accuracy, leading to calculated stability constants that showed strong linear correlations with experimental data across different metal ligand systems. This refined methodology provides a robust predictive framework for determining stability constants in cases where experimental data are unavailable and offers a practical pathway for computational screening of metal-ligand systems in aqueous environments.

P60

A modular classical density-functional framework for gas adsorption in nanoporous materials: from first-principles binding energies to kinetic molecular sieving

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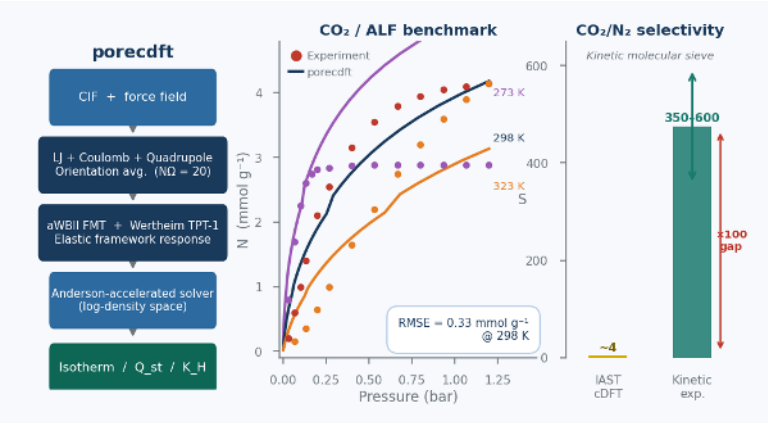
Current computational approaches—rigid-host Monte Carlo and one-dimensional classical density functional theory (cDFT)—cannot quantitatively predict cooperative pore filling, framework flexibility, or kinetic molecular sieving in nanoporous hosts. We present `porecdft`, a modular three-dimensional cDFT framework that combines an orientation-averaged composite external potential (Lennard–Jones + Gaussian-smeared Coulomb + quadrupole–electric-field-gradient), advanced White-Bear II fundamental measure theory with Wertheim first-order thermodynamic perturbation theory (TPT-1) site association, an elastic framework response, and an Anderson-accelerated solver. Demonstrated on the CO_2/aluminum-formate (ALF) benchmark of Evans et al. (*Sci. Adv.* 2022), the framework reproduces the periodic-DFT binding energies at both small (-48 vs -48.4 kJ mol^{-1}) and large cavities within 1%, the 298 K isotherm with a root-mean-square error (RMSE) of 0.33 mmol g^{-1}, and the experimental calorimetric isosteric-heat band (25–32 kJ mol^{-1}). The anomalous experimental temperature ordering $N(323\ \mathrm{K}) \approx N(298\ \mathrm{K}) \gg N(273\ \mathrm{K})$ is identified as a kinetic effect of formate-linker librations directly observed in ab initio molecular dynamics, while the cDFT CO_2/N_2 Ideal Adsorbed Solution Theory (IAST) selectivity of $\sim$4 lies two orders of magnitude below the experimental kinetic value of 350–600, confirming ALF as a kinetic molecular sieve whose selectivity arises from transport rather than equilibrium. As a second benchmark, the framework is applied to H_2 adsorption in four metalated covalent organic frameworks (COF-301, COF-322, COF-330, COF-333) loaded with five first-row transition metals using Morse external potentials; cobalt gives the highest Henry-regime uptake in every COF owing to its broad, soft Morse well rather than its well depth, a result requiring 3D treatment to capture.



P61

The effects of dispersion damping and three-body interactions for accurate layered-material exfoliation energies

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Accurate predictions of exfoliation energies and lattice constants of layered materials hinge on a correct description of London dispersion physics. Modern a posteriori dispersion corrections in density-functional theory (DFT), such as the exchange-hole dipole moment (XDM) model, capture the proper asymptotic behaviour at long range while making use of damping functions to prevent unphysical divergence at short range. In the united-atom limit, the dispersion energy is damped to a finite, non-zero value by both the canonical Becke–Johnson (BJ) damping function and the new Z-damping function. XDM(BJ) has previously demonstrated exceptional accuracy for modelling layered materials, such as in the LM26 benchmark, which includes graphite, hexagonal boron nitride, lead(II) oxide, and transition-metal dichalcogenides. This work presents the first assessment of XDM(Z) on the same benchmark. We also show that inclusion of three-body interactions via the Axilrod–Teller–Muto (ATM) term further improves the computed exfoliation energies for both XDM(BJ) and XDM(Z), yielding the best performance achieved on LM26 using semi-local functionals to date.

P62

Crystal Structure Prediction of Candidate Energetic Materials: Mapping Polymorphic Energy–Density Landscapes

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Crystal packing plays a central role in determining the properties of energetic materials, as the arrangement of molecules in the solid state controls crystal density, detonation performance, and mechanical sensitivity. Crystal structure prediction (CSP) provides a way to assess candidate energetic materials before synthesis by mapping their crystal energy landscapes and identifying low-energy polymorphs. In this work, CSP was used to investigate three borazine-based candidate molecular explosives. A hierarchical workflow was employed, combining large-scale force-field searches across experimentally common space groups with dispersion-corrected density-functional theory to refine lattice energies and optimize promising crystal structures. The resulting crystal energy landscapes predict that one candidate, bearing azido substituents on the heteroaromatic ring, should have a density comparable to that of established CHNO-based explosives, making it a promising target for future synthesis. Overall, the results demonstrate how CSP can focus experimental efforts on the most viable candidates, underscoring the promise of computational screening in the design of new energetic materials.

P63

Quantum-derived molecular fingerprints using Hamiltonian simulation for data-driven coupled-cluster approach

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In quantum chemistry, Coupled-Cluster theory is used to solve the electronic Schrödinger's equation and obtain accurate energies of molecular systems. Solving the coupled-cluster equations requires iteratively finding the optimal one-electron (t_1) and two-electron (t_2) excitation amplitudes. However, obtaining these parameters scales greater than O(N^6), creating a significant computational bottleneck that limits the method's applicability to large molecular systems. To address this, the Data-Driven Coupled-Cluster (DDCC) approach was developed to accelerate the computation of t_1 and t_2 amplitudes by utilizing a machine learning framework that only requires input features derived from relatively cheaper quantum chemistry methods to directly predict the optimal excitation amplitude values. These predicted excitation amplitudes can then be used to efficiently obtain accurate correlation energies at the Coupled-Cluster Singles and Doubles (CCSD) level of theory by either serving as an optimized initial guess for the iterative process ("exact CCSD") or be introduced directly into the energy expression for CCSD ("approximate CCSD). In this context, Quantum Machine Learning (QML) models offer a powerful alternative to classical models in the DDCC approach for predicting these amplitudes and aligning with the quantum-centric supercomputing paradigm. Since the performance of any ML model is heavily dependent on its input features, we are developing Hamiltonian simulation based algorithms as a means to generate high-fidelity quantum-derived input features, or quantum fingerprints. Our work explores the idea of feeding these quantum-derived features into QML models to predict the t_1 and t_2 amplitudes and benchmark the performance for both exact and approximate CCSD correlation energies. Our approach has the potential to enable the estimation of CCSD-quality energies with significantly reduced iterative overhead and providing a methodology for high-level molecular property predictions on emerging quantum architectures.

P64

A Revised Implementation of the SM12 Continuum Solvation Model Targeting Structure, Reactivity and Spectroscopic Applications

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Continuum solvation models are powerful tools for the modeling of condensed phases, and hence for approaching a realistic representation of complex chemical systems in a manner that is tractable for accurate quantum-chemical simulations. The SM12 solvation model, originally proposed by Marenich et al.[1], is a Generalized-Born-Approximation (GBA) based solvation model. SM12 (and other GBA approaches) incorporate electrostatic effects as polarization energy due to partial charges while addressing non-electrostatic effects of the first-solvation shell in the form of atomic surface tension terms.[2] Unique to SM12 among GBA approaches is the use of partial atomic charges that are basis-set independent and are derived from the accurate charge density. SM12 works in combination with the Hirshfeld-derived Charge Model 5 (CM5), and the ESP-derived Merk-Kollmann (MK) or ChElPG charges affording solvation energies for any element in the periodic table. The charge model 5 (CM5)[3] variant was previously implemented for SM12 into the ADF code.[4] However, the CM5 charges are not well-behaved for gradient evaluations, while the analytical gradients of the ESP-derived charges on a Cartesian grid are too expensive. In this contribution, we present a revised SM12 implementation that uses Lebedeev grids to compute ESP-derived charges.[5] These are atom-centered CHELPG (a-CHELPG) charges, that are computationally inexpensive, and well-behaved for energies and gradients. As a result, geometry optimizations are now feasible, and agree with finite-difference numerical gradients for molecules encompassing main-group, transition-metal, and f-block elements. In gas phase, the a-CHELPG charges yield dipole moments that are similar in scale to those from Cartesian grids. An assessment of the different charge options to compute solution-phase vertical excitation energies with SM12 will be presented.

P65

Quantum Chemical Investigations of Fundamental Interactions in Physisorption: Methane/Carbon Materials

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Fundamental understanding of gas physisorption is essential for energy storage, transport and utilization. Natural gas (mainly methane) is an attractive energy resources due to its high energy density and low carbon intensity. A detailed understanding of methane/surface interactions is important for improving methane storage in porous materials. Here, we are developing quantum-level descriptions of these interactions in models of porous carbon systems. Using high-level quantum theories (CCSD(T)/def2-QZVPPD with DLPNO and/or F12 approximations) as benchmarks, we evaluated 90+ DFT functionals on representative examples for methane and porous carbon adsorption models. Five accurately performing DFT functionals were selected to describe a network of C–H...π H-bonding and π...σ^* (C–H), and C–H...σ^* (C–H) tetrel interactions at reasonable computational costs. Computational maquettes were established in order to capture methane adsorption structures and energetics on open carbon surfaces (>15 Å), in between small (7 Å) and large (11 Å) pores. The experimental isosteric heat of adsorption can be estimated from the linear combinations of methane binding energies in various pore sizes. This work provides useful guidance for the experimental design of adsorbent materials. The modeling strategy is being extended to other gases, including H_2, CO_2, and NH_3, as well as to more realistic adsorbent surface models with curvature, surface defect, and presence of heteroatoms.

P66

Mechanistic Insights into Proton Transport in Phosphonate-Based Hydrogen-Bonded Organic Frameworks Using Grand Canonical Monte Carlo and Ab Initio Molecular Dynamics

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University of Alberta

Hydrogen fuel cells offer a promising route toward low-emission energy conversion, as they generate water as a benign byproduct. Their performance critically depends on the proton exchange membrane (PEM), which must combine high proton conductivity with thermal and chemical stability under operating conditions. This has motivated the search for solid-state proton-conductive materials, among which hydrogen-bonded organic frameworks (HOFs) have recently emerged as attractive PEM candidates due to their intrinsic hydrogen-bond networks that can support water-mediated proton transport. Phosphonate-based HOFs are particularly appealing because strong hydrogen bonding between phosphonic acid groups enhances structural stability under ambient conditions. Two such frameworks, UPC-H5a and GTUB-5, have been reported to exhibit high proton conductivities via a Grotthuss-like mechanism, yet UPC-H5a outperforms GTUB-5 by roughly four orders of magnitude. This work aims to clarify how nanoconfinement modulates hydrogen bond network dynamics and, in turn, proton transport, thereby providing a mechanistic explanation for this striking disparity.

We first employed Grand Canonical Monte Carlo (GCMC) simulations and isosteric enthalpy calculations to characterize water adsorption in both frameworks. Despite comparable accessible pore volumes and similar adsorption enthalpies over a wide loading range, GTUB-5 exhibits higher water uptake at intermediate to high pressures, indicating that neither pore volume nor overall adsorption capacity alone accounts for the conductivity differences. To uncover the relevant microscopic factors, we performed Ab Initio Molecular Dynamics (AIMD) simulations to probe the hydrogen bond network within the hydrated frameworks. In UPC-H5a, water molecules approach phosphonate oxygen atoms more closely and form a more persistent yet dynamically reconfiguring hydrogen bond array than in GTUB-5, with frequent hydrogen bond breaking and reforming, which are hallmarks of Grotthuss-type proton transport. These results show that differences in pore geometry and the resulting nanoconfinement control the structure and dynamics of the hydrogen bond network, providing a molecular-level rationale for the superior proton conductivity of UPC-H5a over GTUB-5 and offering design principles for next-generation solid-state PEM materials.

P67

A data-driven approach for computational modeling and prediction of warhead reactivity in designing targeted covalent inhibitors

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We introduce a computational workflow for predicting the reactivity of covalent drug warheads with nucleophilic amino acid residues. Covalent inhibitors form permanent chemical bonds with the target protein through well-defined reaction mechanisms, and accurate prediction of their reactivity is crucial for drug design. This reactivity can be quantified by accurately estimating the reaction barrier heights, which require high-level quantum mechanical (QM) methods that have a prohibitive computational cost. To overcome this challenge and to fill the gap in the availability of a relevant barrier height reference data, I will show how we develop an automated quantum chemical workflow for generating a diverse dataset of reaction barrier heights comprising representative covalent warhead-nucleophile systems. We focus on diverse warhead functional groups and key reaction classes relevant to covalent drug design, including Michael addition, nucleophilic addition, nucleophilic substitution, and others involving biologically relevant nucleophiles. I will further discuss how this dataset will serve as a foundation for in-house developments of data-driven models, including Δ-machine learning approaches that aim to predict corrections to low-level reaction barrier heights with near high-level QM accuracy at significantly reduced computational cost. Overall, I will highlight how our approach provides a computational framework for predicting the reactivity of targeted covalent inhibitors as well as means to generate high-quality datasets that can ultimately facilitate high-throughput prediction for the in silico design of covalent therapeutics.

P68

Accelerating hybrid algorithms for electronic structure calculations

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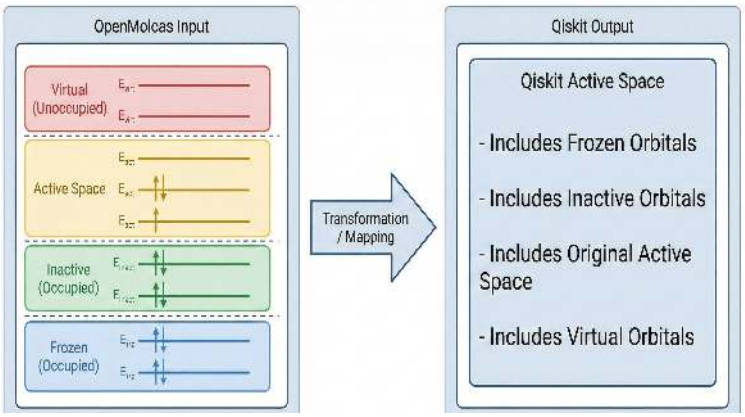
While quantum algorithms offer a promising route to solving complex electronic structure problems, practical implementations on near-term hardware are severely bottlenecked by the scaling of system size. Specifically, the number of optimization iterations required for the variational quantum eigensolver to converge grows exponentially with system size. This scaling crisis can be attributed to two main factors: (1) the vastness of the search space, which makes it more likely to get trapped in local minima or barren plateaus, and (2) the huge number of ansatz parameters, which makes each iteration more expensive.

In this work, we introduce a hybrid classical-quantum workflow to systematically overcome these limitations. First, we generate a high-quality initial ground-state wavefunction using classical pre-computation with OpenMolcas software, which is then refined using a quantum emulator with customized Qiskit libraries. Second, we accelerate the convergence of the quantum optimization by dynamically discriminating and updating only the most impactful ansatz parameters. This presentation will detail our methodology and provide quantitative results for the speed-up achieved by our hybrid algorithm, highlighting strongly correlated molecular systems.



P69

Reconstructing Local Potentials from Matrix Representations in Arbitrary Basis Sets

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Local potentials are routinely represented as matrices in finite basis sets. The inverse problem of recovering a real-space potential from its matrix is widely considered ill-posed. We show that this inverse problem admits a clean and robust solution when products of basis functions are treated as an overcomplete spanning set and their linear dependencies are properly exploited. The resulting method converges to the exact real-space potential in the basis-set limit and efficiently handles very large basis sets on standard desktop hardware. The findings provide a rigorous foundation for potential reconstruction and have direct implications for a wide range of electronic-structure applications involving local operators.

P70

Exploring the hydrogen bonding effects on the structural and energetic properties of gatifloxacin-water aggregates

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In this study, we examined how interactions between solvent molecules and various sites on gatifloxacin (GFX) affect the stability and photoexcitation of the system. The ground- and excited-state properties of protonated and deprotonated GFX surrounded by (up to) six explicitly included water molecules (GFX···$6H_2O$) were calculated using density functional theory (DFT) and time-dependent DFT (TD-DFT), employing two exchange-correlation functionals (CAM-B3LYP and M06-2X) and three basis sets: 6-311++G(d,p), aug-cc-pVTZ, and def2-TZVP. Implicit solvation effects were modeled with the polarizable continuum model (PCM). Comparison with recent results for isolated GFX indicated that hydrogen bonding with water molecules plays a crucial role in stabilizing the deprotonated form of GFX and in modulating the photoexcitation of the protonated species. For example, at the CAM-B3LYP/def2-TZVP level in water, a red shift of ≈ -0.07 eV was observed in the first open singlet excited state of GFX···$6H_2O$ relative to the corresponding result obtained for GFX with only implicit solvation. This shift is likely due to hydrogen bonding interactions within GFX···$6H_2O$.

P71

Constrained Crystal Structure Prediction

Grace Sparrow[1], R Alex Mayo[2], and Erin Johnson[1]

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[2] *XtalPi Inc*

The aim of crystal structure prediction (CSP) is to identify, based on first-principles calculations, the most probable polymorph(s) of a compound to be observed experimentally. The structure generation stage of CSP typically leads to the generation of hundreds of thousands of candidate structures across multiple space groups. For cases where experimental powder X-ray diffraction (PXRD) data is available, but the crystal structure is not yet solved, we propose using indexed lattice parameters to constrain the search space. Searching only specific unit cell dimensions allows a large reduction of the number of structures generated, whilst adding confidence that the experimental structure remains in the search pool. Examples are shown for the cases of several small organic molecules, including urea, uracil, paracetamol, progesterone, and ROY.

P72

Calculate what is measured. Measure what is calculated.

Robert Szilagyi

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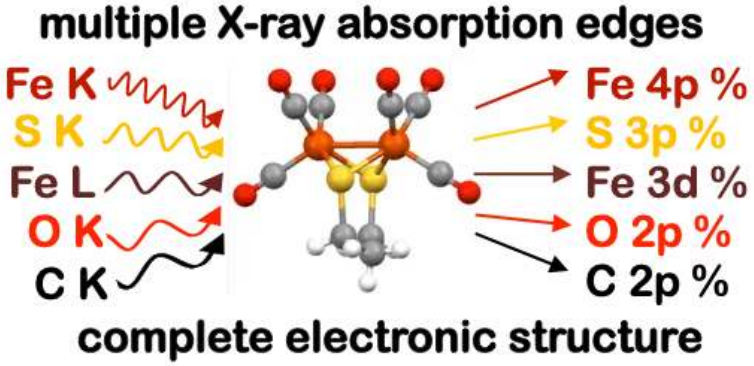
The presentation will be an invitation for expanding the repertoire of any computational chemist with research interests in electronic structure information, such as orbital composition (covalency), Coulomb interactions (effective nuclear charge), exchange interactions (spin polarization), for organic, inorganic, and organometallic compounds. The rainbow of X-rays employed in multi-edge X-ray absorption spectroscopy is an established high-energy physics technique



for developing density functionals, refining empirical potentials for tight-binding methods, validating basis sets with high-level ab initio wave function methods, to name a few applications that we have been directly or indirectly involved through collaborations. Selected “classical” examples will be highlighted for the complementary information content of synchrotron-based spectroscopy in addition to hot-off-the-beamline results obtained at the Canadian Light Source during our May 2026 beamtime trip.

P73

Grid-Based Quantum Simulation of Vibrational Hamiltonians and Pyrazine Vibronic Spectra

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Using grid based representation in classical tensor product by increasing the dimension of system is expensive. Thanks to Quantum simulations, this approach can make advantages compared to the classical systems. This research aims to present a mesh-based qubit-operator framework for solving the time-independent Schrödinger equation. We begin with a formulation, the diagonal operator which encodes the mesh coordinate and generates the potential term and the shift operators which generate the nearest-neighbor couplings associated with the kinetic energy operator. The framework is validated on harmonic and anharmonic benchmark potentials using exact diagonalization, the Variational Quantum Eigensolver, and Variational Quantum Deflation. The accuracy of the method is evaluated through energy errors, energy quotients, and wave-function fidelities. We further extend the approach to a molecular vibronic Hamiltonian for pyrazine, where vibrational modes are encoded on qubit grids and coupled to an electronic-state qubit. Quantum phase estimation is then used to extract spectral weights and construct the absorption spectrum. The results demonstrate that the proposed qubit-grid representation provides a flexible framework for simulating continuous-variable quantum systems, molecular vibronic Hamiltonians, and related quantum dynamics problems on quantum computing platforms.

P74

Transformer Variational Autoencoder with Latent DDPM Flow Matching for Synthetic Molecular Generation

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Molecular generation is an important task in computer-aided drug discovery, where deep generative models can be used to explore novel chemical structures. In this work, we present a molecular generation framework that combines a Transformer-based variational autoencoder with latent flow matching. Molecular structures are first converted from SMILES strings into SELFIES representations to improve syntactic robustness during generation. The variational autoencoder uses a Transformer encoder with class-token pooling to learn continuous latent representations of molecules, together with an autoregressive Transformer decoder for sequence reconstruction and generation. To improve latent-space sampling, a diffusion model utilizing flow matching technique is trained on the learned molecular latent vectors and used to generate new latent samples. Generated molecules are evaluated using standard molecular generation metrics, including validity, uniqueness, novelty, quantitative estimate of drug-likeness, Jenson-Shannon distance across more than 30 chemical properties, and diversity. The results demonstrate that combining attention-based molecular representation learning with latent flow matching provides a flexible framework for generating chemically valid, diverse, and novel molecular structures. This approach offers a promising direction for molecular design and virtual screening applications.

P75

Machine Learning Methods for Molecular Energy Prediction

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In recent years, different machine learning methods have been proposed for total energy prediction and molecular design. Having a robust architecture and a good descriptor is crucial in neural networks as they can significantly impact the final results. Here we investigate the use of multilayer perceptron neural networks (ReMLP-NET) and transformer encoders (Transformer-Potential) in molecular energy prediction. The methods are trained on a dataset called Retrievium, which mainly contains organic structures with elements H, C, N, O, S, and Cl, originating from the GDB13 dataset. The atomic environment vector is generated based on the symmetry functions used in ANI-2x, where it spans both configurational and conformational space, with the addition of genetic algorithm optimized parameters in the case of ReMLP-NET. Unlike ANI-2x, which includes a separate network for each element, both ReMLP-NET and Transformer-Potential use a single network. Different preprocessing steps are performed on the employed dataset to accelerate the learning process and improve the results. The ReMLP-NET and Transformer-Potential methods are compared with the well-known ANI-2x in terms of total energy, where they obtained results of 1.29 and 1.33 kcal/mol for MAE on average, respectively, compared to 1.53 kcal/mol for ANI-2x.

P76

Effective theory of quantum phases in the dipolar planar rotor chain

Estêvão V.B. de Oliveira[1], Muhammad Shaeer Moeed[1], and Pierre-Nicholas Roy[1,2]

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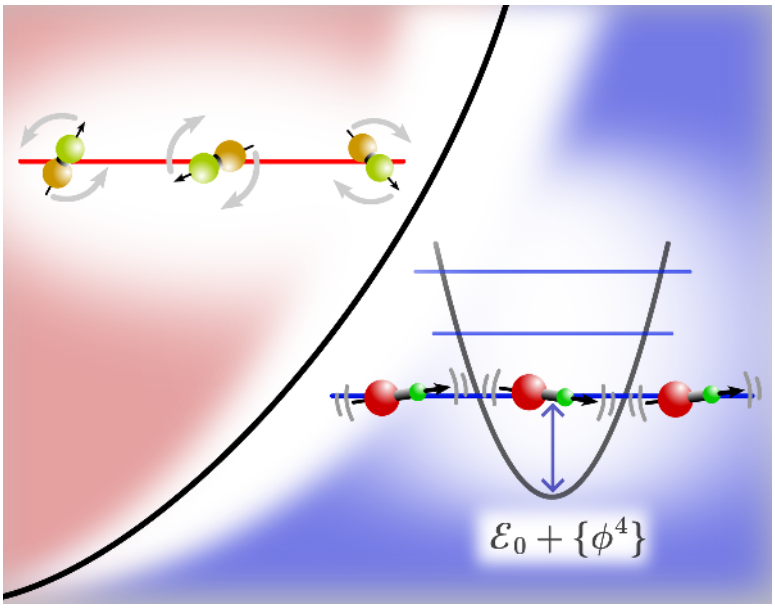
[2] *Department of Chemistry*

In this work, we develop a theoretical description of the collective behavior of interacting dipolar planar rotors by using time independent perturbation theory and a small angle quadratic approximation. The ground state properties for both the ordered and disordered quantum phases of the system are directly calculated and analyzed. Time-independent perturbation theory is shown to be appropriate for the disordered phase. For the ordered phase, we construct a quadratic approximation based on the stable equilibrium configurations of the dipolar ordering; we show that the inclusion of the quartic terms from the expansion of the potential energy are essential to correct the shift in the energy spectrum due to quantization ambiguities. Numerical techniques such as Exact Diagonalization (ED) and Density Matrix Renormalization Group (DMRG) are used for the benchmark the quality of both approximations.



P77

Sparse and interpretable neural network architecture for scientific data

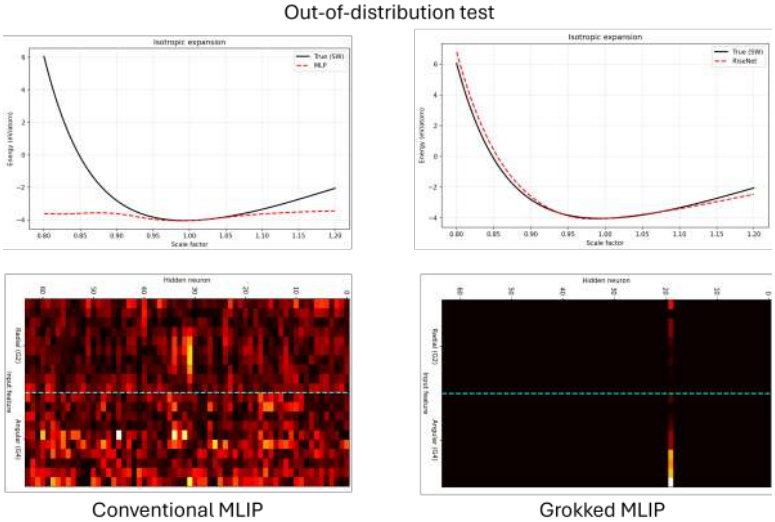
Oleksandr Voznyy

University of Toronto Scarborough

In deep learning, ”grokking” describes a delayed phase transition where a model, after a long period of memorizing training data, suddenly discovers a generalizable solution and test accuracy spikes. To date, this phenomenon has been treated as a curiosity observed primarily in clean, algorithmic tasks (e.g., modular arithmetic). The prevailing dogma in the physical sciences is that grokking is inaccessible for scientific datasets, which are characteristically small, high-dimensional, and inherently noisy. Consequently, most models in computational chemistry—from property predictors to Machine Learning Interatomic Potentials (MLIPs)—operate in the ”memorization” regime, resulting in brittle performance when extrapolating to new out-of-distribution chemical spaces.

Here, we challenge this assumption. We demonstrate a method to accelerate the onset of grokking on arbitrary, noisy datasets. We show that models are compelled to abandon ”shortcut learning” (memorizing noise) in favor of ”structural understanding” (learning the underlying physics). We demonstrate the implications of this approach for materials science: enabling the training of robust MLIPs that maintain stability outside their training domain and extracting physical laws from sparse, noisy experimental data.

This work suggests that the ”Small Data” problem in science is not a lack of information, but a failure of the training dynamics to access the generalized solution.



P78

Operator Entanglement in Quantum Dynamics Simulations

Tzu Yu Wang, Michael Schuurman, and Simon Neville

University of Ottawa

We review the framework of operator Hilbert space and introduce the one- and two-particle super reduced density matrices (1-SRDMs and 2-SRDMs), as well as the super mutual information (SMI). The eigenvectors of the 1-SRDMs define what we term natural single particle operator bases, which provides a way to compress vibrational and vibronic Hamiltonians with controlled error. The SMI is defined from the operator entanglement entropy of the 1-SRDMs and 2-SRDMs, and captures the correlation between operators acting on different one-mode subspaces, and may be used to reveal and quantify both direct and indirect couplings that might otherwise be difficult to extract. These analysis tools are applied to a set of prototypical vibrational and vibronic Hamiltonians, as well as approximations to the corresponding time-evolution operators. Through this, we demonstrate that: (i) commonly used vibronic Hamiltonians are amenable to extremely high levels of compression without compromising accuracy, and; (ii) SMI analysis can be used to systematically and quantitatively reveal both direct and indirect couplings that might otherwise be difficult to extract, including indirect couplings of vibrational modes via intermediary electronic-vibrational interactions.

P79

Generative ML of 3D-periodic Materials using a Novel Invertible and Invariant Graph Encoding

Andrew White and Tom Woo

University of Ottawa

Generative machine learning (ML) for materials discovery requires a way of representing a chemical system (an encoding) which is compatible with modern ML algorithms. To facilitate training, the encoding should satisfy the conditions of invertibility (that the encoding can be interconverted between human-interpretable and machine-interpretable formats without loss of information) and invariance (that each unique structure corresponds to a unique encoding irrespective of coordinate transformation, preventing data leakage and accelerating training). While invertible, invariant representations for molecules such as SMILES have been developed and deployed (e.g. in drug design and discovery), this remains an open problem for periodic structures, where periodic boundary conditions add unique challenges. Current state-of-the-art methods for periodic structures explicitly encode the lattice vectors and/or periodic boundary, and are therefore not invariant to the choice/orientation of lattice vectors. Here, we present an alternative approach where geometry is encoded as internal coordinates (bonds, angles, torsions) while lattice vectors and periodic boundaries are not encoded. This approach ensures full roto-translational invariance, while lattice vectors and periodic boundary conditions remain recoverable as an emergent property of the underlying system. Generation of novel materials under this encoding entails sampling the composition (number and type of atoms), connectivity (number and type of bonds) and geometry (encoded as internal coordinates). We adopt a modular approach, with independent models trained for each generative task. The design and implementation of the graph encoding and decoding tool will be discussed, as well as the development of diffusion-based connectivity and geometry models. Limitations of and avenues for future developments of both the encoding and generative models will be discussed.

P80

Modelling molecular rotations with analog quantum computing

Siri Williamson and Ryan MacDonell

Dalhousie University

The development of quantum technology over the last few decades has opened new pathways to solving more complex computational problems. While the goal of a universal, fault-tolerant quantum computer is still out of reach, success has been found with modelling quantum chemical systems with analog quantum simulators. Analog quantum simulators are dedicated devices restricted to simulating a limited class of quantum systems: the evolution of the desired quantum system is mapped onto the controlled evolution of the simulator.

Developing an algorithm for rotational motion lays the foundation for modelling more complex dynamics, such as coupling between rotational and vibrational modes. This phenomenon, known as Coriolis coupling, is crucial in computing accurate rovibrational spectra, which are used to identify molecules present in the interstellar medium. Classical methods are limited by requiring numerical approximations or high-quality experimental spectra to use as refinement data.

We have developed the first quantum algorithm for the simulation of rigid rotors. Our algorithm is adapted for present-day quantum simulators by using two vibrational modes to represent rotational modes. We show that our algorithm can produce accurate rotational spectra for different types of rigid rotors. This allows for the addition of vibrational modes for exact computation of Coriolis coupling. Future work includes using a non-rigid rotor model, which will allow for simulation of floppy molecules with more complex internal dynamics.

P81

Fast Estimation of Kinetic Correlation in Density-Functional Approximations

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Approximations to the Kohn–Sham exchange-correlation functional contain an unknown and uncontrolled contribution: the kinetic correlation energy, T_c. Standard extraction methods require evaluating functional derivatives and integrating via the Levy–Perdew virial relation, which is computationally demanding. We investigate a simpler estimation formula that would not generally be expected to perform well for approximate functionals, yet proves remarkably accurate in practice.

P82

High-throughput computational screening of metal organic framework database for membrane separation of C3H8/C3H6 mixture

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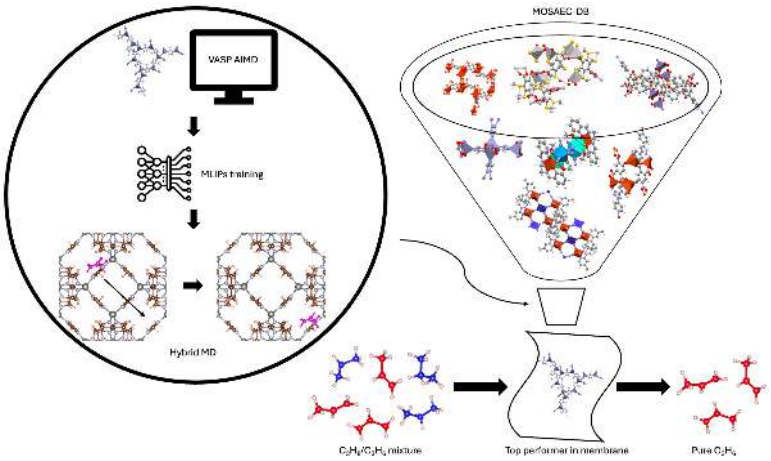
Current industrial alkane/alkene separations rely on energy-intensive distillation-based technologies, with C2 and C3 separations alone estimated to account for approximately 0.3% of global energy consumption.1,2 The separation of propylene (C3H6) from propane (C3H8) is particularly challenging due to their near-identical boiling points, similar molecular sizes, and extremely close relative volatility, yet it remains critically important given propylene's widespread use as a petrochemical feedstock.3 Metal-organic frameworks (MOFs) — porous materials composed of inorganic metal nodes and organic linkers connected by coordination bonds — offer a promising alternative to conventional separation methods. In this work, we investigate MOF-based membrane separation, where gases are distinguished by differences in their diffusion and adsorption coefficients as they permeate through the framework. Guest molecules with stronger host–guest interactions diffuse more slowly, enabling selectivity. Key performance metrics screened in this work include diffusion coefficient, permeability, and membrane selectivity. MOFs were sourced from the MOSAEC database.4 An initial geometric filter based on pore-limiting diameter (PLD ≥ 2.9 Å) reduced the working dataset from 106,553 to 28,729 structures. Grand Canonical Monte Carlo (GCMC) simulations were then performed to identify top-performing adsorbers for further study. To model framework flexibility — which is critical for MOFs such as ZIF-8 and CALF-20 that are experimentally known to separate propane/propylene mixtures — we employ a hybrid interatomic potential approach. Machine learning interatomic potentials (MLIPs), trained on periodic DFT calculations using DeePMD-kit, capture the dynamic flexibility of the MOF host, while classical Lennard-Jones (LJ) potentials describe guest–guest and host–guest interactions.5,6,7 LAMMPS molecular dynamics (MD) simulations are then used to compute guest diffusion. As a proof of concept, this hybrid framework has been validated for CO2 diffusion, demonstrating its ability to recover physically meaningful transport behaviour in flexible MOFs. Extending this methodology to C3 mixtures in ZIF-8 and CALF-20 is currently underway, with the goal of identifying selectivity trends that can guide the design of next-generation membrane materials.



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P83

A diabatization and electron-phonon coupling Hamiltonian construction protocol for periodic systems

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Time-dependent density functional theory (TDDFT) is a daily tool for exploring excited states in materials science for its compromise of accuracy and efficiency. It provides information of energies and transition patterns of excited states. TDDFT only provides adiabatic states that can evolve abruptly along nuclear distortion, since the building blocks of the method are the adiabatic Kohn-Sham orbitals. The hole-particle pairs involved in an excitation can be viewed as an image of the wave function of the excited state. With the transition density that is made of such pairs and contains information of hole-particle correlation, we developed a diabatization protocol to decompose the TDDFT excited states into diabatic states that maintain their electronic character regardless of nuclear distortion. This protocol helped characterize intralayer local excitons and interlayer charge-transfer excitons in our recent study of different stackings of silicane (SiH). This protocol also enables construction of diabatic electron-phonon coupling Hamiltonian. With a so-constructed Hamiltonian and using the augmented fewest switch surface hopping (AFSSH) nonadiabatic dynamics, we explored the transition time scale from direct band gap transition to indirect band gap transition of SiH, which is of critical importance in determining the utility of this class of 2D nanomaterials in optoelectronics, as good candidates in light emitting, photovoltaics, or photocatalysis.