Canadian Symposium on Theoretical and Computational Chemistry (CSTCC2024)

[#CSTCC2024]

Book of Abstracts

hosted at

DALHOUSIE
UNIVERSITY

July 21-25, 2024

Canadian
Association of
Theoretical
Chemists

Association
Canadienne des
Chimistes
Théoriciens

Welcome Message

We are happy to welcome you to the 30th Canadian Symposium on Theoretical and Computational Chemistry (CSTCC2024), which is the premier biennial event of the Canadian Association of Theoretical Chemists (CATC) and the largest meeting of theoretical and computational chemists in Canada. The 30th CSTCC will be hosted in 2024 by Dalhousie University, continuing the tradition of bringing together researchers from Canada and around the world.

The organizing committee

Erin Johnson [Dalhousie]
Ryan MacDonell [Dalhousie]
Stijn De Baerdemacker [UNB]

Contents

Program at a glance

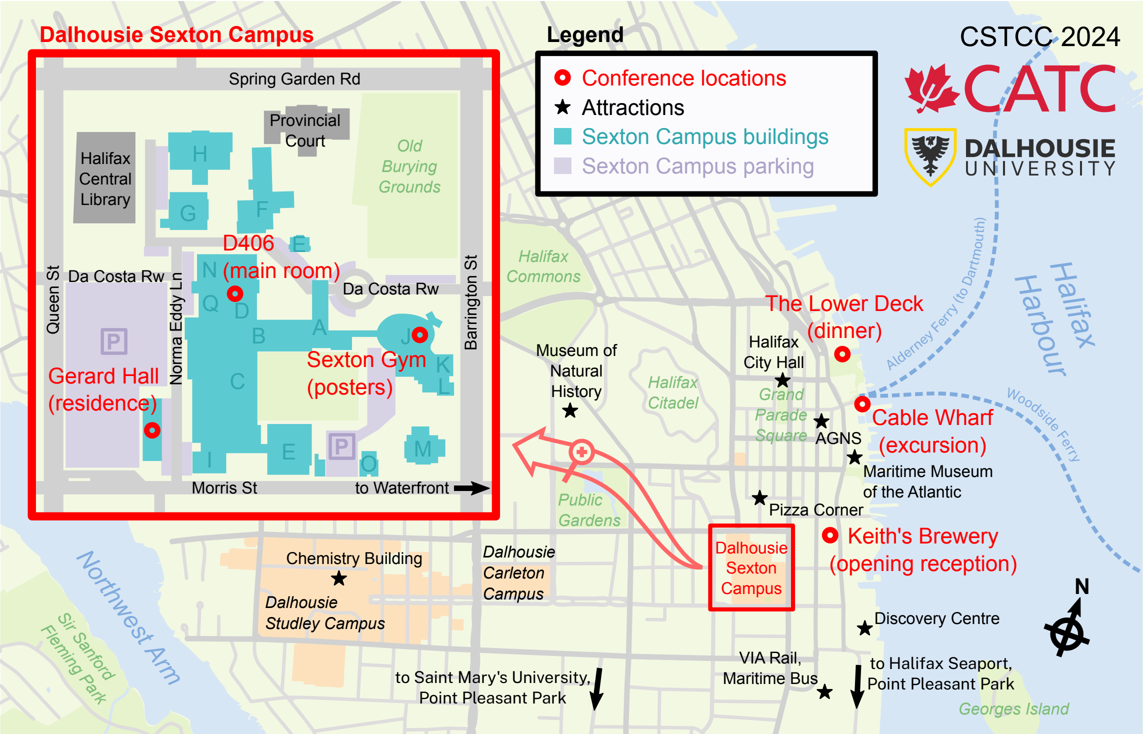
SESSION TITLE
{*Chair*}
Speakers

time	Monday 22/07	Tuesday 23/07	Wednesday 24/07	Thursday 25/07
09h00	DFT DEVELOPMENT {*Hollet*} Burke Gerolin	PLENARY {*Boyd*} Becke Staroverov	CATC LECTURE {*Woo*} Ayers (CATC) Bultinck	BIOCHEMISTRY {*Wiebe*} Gentile Gauld
10h15	Break	Break	Break	Break
10h30	INTERMOLECULAR {*Wetmore*} DiLabio Herbert Hernández Trujillo	CONDENSED MATTER {*Bowles*} Zwanziger Zurek Blum	WAVEFUNCTIONS {*Heidar-Zadeh*} Johnson Piecuch Thompson	SOLID STATE {*Chen*} Paci Beran Tetsassi Feugmo
12h00	Lunch	Lunch	Lunch	Lunch
13h30	NONADIABATIC {*Brown*} Maitra Izmaylov Zeng	MACHINE LEARNING {*Pearson*} Voznyy Vargas-Hernández Price [CT] El-Samman [CT]	QUANTUM COMPUTING {*Baker*} Head-Marsden Degroote Kottmann	LIGHT-MATTER {*Schuurman*} Autschbach Blaskovits Worth
15h00	Break	Break	Break	Closing
15h15	CONTRIBUTED TALKS {*Mora-Diez*} Leal-Sánchez Ha Yaghoubi Jouybari Ayati Bryenton	CONTRIBUTED TALKS {*Peslherbe*} Meng Javaheri Shamekhi Wang Ghasempouri	CATC MEETING	
19h00	Excursion	Banquet	Poster Session	

Practicalities

Map

All venues are within a 20mins walk within each other's reach. A single `.pdf` of the map can be found here.



Opening Reception & Registration Desk

The opening reception and first-day check-in will happen on the evening of Day 0 (Sun 21/07 | 19h00-21h00)

- Alexander Keith's Brewery
  1496 Lower Water St

Halifax, NS

Conference Venue & Registration Desk

All scientific sessions will take place at

- Dalhousie Sexton Campus
  Building D, room D406 (oral presentations)
  Sexton Memorial Gym, Building J (poster sessions)

Wifi

The Dalhousie Sexton campus is covered by the eduroam network, allowing for convenient online access. Those participants who do not have access to eduroam, are advised to contact the registration desk to receive individual wifi access information.

Excursion

The excursion is planned on the evening of Day 1 (Mon 22/07 | 19h00-21h00), with a boat tour in the Halifax harbour (boarding at 18h30)

- Ambassatours
  Cable Wharf
  1751 Lower Water St,
  Halifax, NS

Banquet

The social banquet is on the evening of Day 2 (Tue 23/07 | 19h00-23h00, drinks at 18h00)

- The Lower Deck
  1887 Upper Water Street
  Halifax, NS

Show your Badge

Halifax is a major city and prime destination on Canada's east coast. In addition to the social activities during the conference (boat!), some major attractions include:Point Pleasant Park, Public Gardens, Halifax Citadel, George's Island, Martime Museum of the Atlantic, Art Gallery of Nova Scotia, etc. When enjoying the local atractions, make sure to let your badges work for you! Discounts across town can be be obtained with the Show your Badge program. More general information about Halifax can be found at discoverhalifax.com.

Sponsors

We gratefully acknowledge financial support from our sponsors.

Students and Early Career Researchers can compete for the *Best Presentation awards*, generously offered by our sponsors .

- Best Poster award
  - 1× [200$ + 200£ voucher]
  - 2× [100$ + 150€ voucher]
- Best Contributed Talk award
  - 200$ + 200£ voucher

Awards will be decided by popular vote from all participants.

Full Program

Day 0: Sunday July 21

19H00-21H00 | OPENING RECEPTION & REGISTRATION DESK

Venue: Alexander Keith's

Day 1: Monday July 22

09H00-09H15 | WELCOME

Room: D406

09H15-10H15 | DFT DEVELOPMENT

Chair: **Josh Hollett** *University of Winnipeg, MB, Canada.*
Room: D406

Elementary considerations in DFT

Kieron Burke *University of California Irvine, CA, USA*
I will discuss some basic notions of density functional theory and the surprising insights that can be drawn from them, including their relevance to machine-learning functionals and density-corrected DFT.

Transporting Reduced Density Matrix Functional Theory away beyond the constraint search

Augusto Gerolin *University of Ottawa, ON, Canada*
In this talk, I will discuss how to compute the exact 1-particle Reduced Density Matrix Functional using a dual-variable approach as well as highlight connections with Quantum Optimal Transport Theory. This approach is practical even for strongly-correlated electrons (where density-matrix functional theory may be expected to surpass density functional theory) and relatively large systems.

10H15-10H30 | BREAK

10H30-12H00 | INTERMOLECULAR INTERACTIONS

Chair: **Stacey Wetmore** *University of Lethbridge, AB, Canada.*
Room: D406

Improving the Accuracy of Quantum Chemistry Methods with Optimized Effective Potentials

Gino DiLabio *University of British Columbia, BC, Canada.*

The perennial challenge in applied quantum chemistry is balancing the computational resources (time, disk, memory) associated with simulation work with the accuracy of the results obtained. Our recent efforts have focused on the development of a modification to approximate density-functional (DFT) and wavefunction theory methods to improve their accuracy to that associated with highly-correlated (and resource intensive) wavefunction theory and experimental results. Our approach, which can be described as a Δ-DFT (or Δ-machine learning) method, is based on optimized atom-centered potentials (ACPs). Unlike machine learning approaches, ACPs can be developed using datasets consisting of as few as 100 data points. The potentials are “shaped” such that they mitigate the errors associated with common computational chemistry methods, including incomplete wavefunction descriptions, poor DFT descriptions of exchange/correlation, delocalization error, and so on. The optimized ACPs are used in conjunction with the computational method for which they were developed and require little – if any - additional computing resources. The ACP concept, development process, their applications and performance will be presented.

How Accurate is DFT for Nanoscale van der Waals Complexes, and what Are the Alternatives?

John Herbert *Ohio State University, OH, USA.*

Advances in dispersion-corrected and dispersion-inclusive density functionals over the past two decades have brought the field to the point where intermolecular interactions in small dimers (ca. 20 atoms or fewer) can be predicted with sub-kcal/mol accuracy, using a variety of approaches that are reasonably consistent with one another. The same is not true of nanoscale van der Waals complexes with 100+ heavy atoms, where errors of several kcal/mol are common and there is far less consistency across different DFT-based methods. For these larger systems, there are also sizable discrepancies between putative ab initio benchmarks. This talk will describe the present status of non-covalent quantum chemistry in supramolecular complexes at the nanoscale.

Ehrenfest Forces and the chemical bond

Jesús Hernández-Trujillo *Universidad Nacional Autónoma de México, CDMX, Mexico.*

The nature of the chemical bond can be directly analyzed in terms of forces. The force exerted on an electron in an atom, molecule or solid is the result of its interaction with the other electrons and the nuclei. This quantum mechanical observable, called the Ehrenfest force, can be analyzed as a vector field density, $F(r)$, which comprises a classical term that accounts for the electrostatic interaction of the electron density plus a quantum mechanical contribution that involves the exchange-correlation density. $F(r)$ is a non-gradient field that allows for a dense partition of three dimensional space and to define molecular structure. In addition, the quantum mechanical exchange-correlation Ehrenfest force density, $F_{\mathrm{xc}}(r)$, is a vector field that depends on the action of Pauli exclusion principle. It accounts for the effect of electron pairing, localization and delocalization, thus providing information concerning the nature of the atomic interactions in a molecule. In particular, with the divergence of $F_{\mathrm{xc}}(r)$ the shell structure of atoms is obtained; polar, covalent and ionic bonding can be also identified, with a remarkable similarity with the properties of the Laplacian of the electron density. Therefore, $F_{\mathrm{xc}}(r)$ and its divergence condense on one electronic coordinate the information carried by the complicated six-dimensional exchange-correlation density via the appropriate space-spin integration, a mapping that allows to analyze the structure of the forces exerted on the electron distribution and the chemical bond in real space.

12H00-13H30 | LUNCH

13H30-15H00 | NON-ADIABATIC PROCESSES

Chair: **Alex Brown** *University of Alberta, AB, Canada.*
Room: D406

Electron-Nuclear Correlation via the Exact Factorization Approach

Neepa Maitra *Rutgers University, NJ, USA*

The exact factorization approach enables the definition of exact potentials driving the dynamics of a quantum subsystem coupled to other quantum subsystems. These potentials yield insight into correlations and provide a useful starting point for new approximate methods e.g. for electronic structure embedding for strong correlation, for mixed quantum-classical dynamics of electrons and ions, and for photon-matter coupling. We briefly review recent progress in these areas, and highlight some success in predictions of exact-factorization-based methods compared with traditional methods, as well as some on-going improvements to the methods. Some of our recent work has focussed on electronic coherences, which are key to understanding and controlling photo-induced molecular transformations. While the evolution of electronic coherences is known to depend on nuclear motion, the exact nature of this electron-nuclear correlation has not yet been well-understood: are inherently quantum aspects of nuclear motion significant, or does an essentially classical picture capture the physics? We discuss the importance of the projected nuclear quantum momenta, and how spatial-resolution influences predictions of experiments even when they measure only spatially-integrated coherences. While traditional trajectory-based simulation schemes are blind to the quantum momenta, exact-factorization-based methods approximate these correlation terms, and correctly capture electronic coherences in a range of situations.

Algebraic techniques for quantum computing in quantum chemistry

Artur Izmaylov *University of Toronto, ON, Canada.*

Quantum chemistry problem is one of the attractive targets for demonstrating quantum advantage of quantum computing technology. Having strongly correlated systems as the main target, I would like to discuss what new classical computing techniques need to be developed to help quantum computing algorithms to solve the electronic structure problem. Encoding the electronic Hamiltonian in the second quantized form on a quantum computer is not a trivial problem, and its efficiency can become a bottleneck for the entire quantum solution. Dealing with this Hamiltonian can be facilitated by partitioning it into a sum of fragments diagonalizable using rotations from either small Lie groups or the Clifford group. These fragments are convenient for performing various algebraic manipulations required in circuit compiling and quantum measurement. I will illustrate how the Hamiltonian partitioning can be used to improve performance of several quantum algorithms for quantum chemistry (e.g. Variational Quantum Eigensolver and Quantum Phase Estimation).

Our recent studies in vibronic coupling: simulation of intramolecular singlet fission

Tao (Toby) Zeng *York University, ON, Canada*

Singlet fission (SF) is a vibronic coupling process that converts one short-lived singlet exciton to two long-lived triplet excitons. It can potentially enhance the power conversion efficiency in photovoltaic devices. In the new concept of intramolecular singlet fission (iSF), chromophore units are covalently bonded, so that it is easier to adjust inter-chromophore morphology to facilitate SF. In this seminar, our recent studies of SF materials are presented. Through using our new diabatization scheme and performing quantum chemistry calculations and quantum dynamics simulations, we designed iSF chromophores through a new strategy of introducing N-oxyl moieties to polycyclic aromatic hydrocarbons. We found a model chromophore, pyrazino[2,3-g]quinoxaline-1,4,6,9-tetraoxide, which undergoes the fastest iSF in 16fs and has the smallest size with only 18 non-H atoms. The small model enabled us to perform the first atomistic simulation of the recombination and found that the $T_1T_1 \rightarrow T_2S_0$ triplet fusion, despite its significant exoergicity, is kinetically hindered by a hidden intersystem crossing. The long believed $E(T_2) > 2E(T_1)$ criterion for designing iSF and SF chromophores shall be abandoned.

15h00-15h15 | Break

15h15-16h00 | Contributed Talks

Chair: **Nelaine Mora-Diez** *Thompson Rivers University, BC, Canada*
Room: D406

Hybrid quantum simulation of the molecular dynamics of the relaxation of LiH without the Born-Oppenheimer approximation.

Edith Leal-Sánchez *Dalhousie University, NS, Canada.*

The molecular dynamics of the relaxation of the LiH molecule is simulated using a wave function ansatz that treats electronic and nuclear degrees of freedom (DOF) on the same footing, known as the pre-Born-Oppenheimer (preBO) ansatz. It takes advantage of the the well-developed electronic structure theory, while still fully accounting for the electron and nuclear entanglement. The common practice of separating the DOFs in dynamical simulations leads to incorrect predictions of the outcomes of photochemical processes involving important excited state phenomena, such as intersystem crossing. Despite this, fully entangled simulations are rarely done, especially for systems with more than two nuclei and two electrons, since the problem quickly becomes computationally intractable if the classical model of computation is used. On the contrary, if the quantum model is used, manipulating quantum states becomes tractable, since the units of computation are quantum systems themselves. This allows for the mapping of the molecular wave functions to the wave function of the quantum bit. However, the hardware required for accounting all the degrees of freedom and operations onto a molecular wave function needed for a fully entangled dynamical simulation will not be available in the near future. Here, we present the development of an encoding for the preBO ansatz in an hybrid manner, that is, using an algorithm that distributes the workload between quantum and classical processors. We follow the progress of the relaxation reaction of the LiH by means of the autocorrelation function, which is also used to calculate the spectrum.

Analog Quantum Simulation of Molecular Vibronic Dynamics in the Pre-Born-Oppenheimer Framework

Jongkwon Ha *Dalhousie University, NS, Canada.*

Understanding molecular vibronic dynamics induced by light-matter interaction is crucial for potential application of photochemical process to designing high-functional molecular devices. However, due to huge computational cost of simulating exact quantum molecular vibronic dynamics, majority of the simulation methods relies on the Born-Oppenheimer (BO) approximation, which separates the nuclear and electronic degrees of freedom, to at least some extent which may cause inaccuracy originated from the basis set truncation. On the other hand, quantum computing can efficiently perform quantum dynamics simulation by utilizing quantum mechanical features of the computing device. Nevertheless, existing quantum simulation methods in quantum chemistry and NAMD still rely on the BO framework. In this work, we present a novel analog quantum simulation approach for molecular vibronic dynamics in the pre-BO (pre-BO) framework which do not separate the nuclear and electronic degrees of freedom using coupled multi-qubit-boson mapping based on the second quantization representation. The electronic state in the second-quantized pre-BO representation of the molecular state spans the complete basis set space for a given orbital basis set, i.e. the full configuration interaction space. We show that our approach has a linear scaling with respect to the number of nuclear degrees of freedom or electronic orbitals, which is significantly reduced compared to the equivalent simulation on classical computers.

Computing Non-Adiabatic X-ray Absorption Spectra of Ethylenic Molecules Using a Vibronic Coupling Hamiltonian

Martha Yaghoubi Jouybari *University of Ottawa & NRC, ON, Canada.*

Advancements in ultra-fast X-ray sources now offer unprecedented capabilities in X-ray spectroscopy, providing high-quality data that demands increasingly sophisticated computational methods for analyzing and interpreting experimental results. One key challenge lies in understanding the interplay between electronic transitions and vibrational motion, known as vibronic coupling. This interaction influences X-ray absorption spectra (XAS) by broadening and shifting absorption peaks, leading to the observed fine structures. Simulating XAS poses a significant challenge due to the requirement to consider a large number of excited states. As energy increases, the excited state manifold becomes denser, ensuring the existence of strong vibronic coupling between excited states. In the realm of XAS, vibronic coupling significantly influences spectral features. Our study aims to investigates the impact of vibronic coupling on the XAS of Ethylenic Molecules . To achieve this, we employed Quantum Dynamics (QD) simulations based on a vibronic coupling Hamiltonian. For the quantum dynamics calculation, we employed the Multi-Configuration Time-Dependent Hartree (MCTDH) method using the MCTDH package. The simulation results underscore the crucial role of incorporating vibronic coupling to accurately reproduce the experimental XAS spectrum.

Spin Symmetry Breaking in Electronic Structure Theory

Amir Ayati *University of New Brunswick, NB, Canada.*

In a Hartree-Fock (HF) calculation, breaking the spin symmetry by permitting electron unpairing can lead to qualitatively superior energies near bond dissociation. I will present a method built on this spontaneous spin symmetry breaking associated with bond-breaking processes to address strong electron correlation in molecular systems. In our method, a constrained-unrestricted-HF (c-UHF) approach is used to break the spin symmetry for any given system, allowing the generation of states with specific spin expectation values. Subsequently, these spin-contaminated states are used in a non-orthogonal Configuration Interaction (NOCI) expansion to restore the spin symmetry and capture the missing correlation. Two different approaches for constructing the NOCI basis were developed. (1) the spinGCM; a linear combination of c-UHF states is chosen in the Generator Coordinate Method (GCM) framework. (2) the SpinProjection; spin symmetry is restored with the aid of projection operators in a projection-after-variation (PAV) manner. Both approaches were tested on different molecules exhibiting static and/or dynamic correlation and were proved effective in capturing the missing correlation, especially where static correlation predominates.

Adding Correlation to the Exchange-hole Dipole Moment Model

Kyle Bryenton *Dalhousie University, NS, Canada.*

Density-functional theory (DFT) allows first-principles computational modelling of the electronic structure of large-scale quantum systems. The combination of DFT's high efficiency and accuracy has positioned it as the workhorse of computational chemistry in recent years. Standard DFT methods neglect dispersion, a weak intermolecular force that determines properties like friction, adhesion, crystal structure packing, and the shapes of biomolecules. To capture dispersion interactions, we incorporate corrections such as the exchange-hole dipole moment (XDM) model. In recent studies, we demonstrated that XDM correctly captures dispersion physics and exhibits best-in-class performance on a benchmark of 15,000 chemical systems. Rather than using exact exchange, most implementations of the XDM model use the localized Becke-Roussel (BR) hole to calculate the exchange-hole dipole moments. This choice of model hole is more computationally efficient, especially for solid-state systems, while also capturing non-dynamical correlation from chemical bonding, thereby improving accuracy for many molecular systems. However, this approach fails to capture short-range dynamical correlation, which we now add using the real-space model of Becke. Here, we present the mathematical framework, implementation in FHI-aims, and benchmarking of the exchange-correlation-hole dipole moment model (XCDM).

19H00-21H00 | EXCURSION

Day 2: Tuesday July 23

09H00-10H15 | PLENARY

Chair: **Russel Boyd** *Dalhousie University, NS, Canada.*
Room: D406

My COVID project: GMTKN55, a new hybrid density functional, and (nooooo, say it isn't so!) a new double hybrid functional

Axel Becke *Dalhousie University, NS, Canada.*

The GMTKN55 (general main-group thermochemistry, kinetics, and noncovalent interactions) chemical database of Goerigk, Grimme, and coworkers [1] is a compilation of highly accurate computed reference data for 1505 chemical reactions in 55 subsets representing diverse types of chemistry. Since 2022, we have used GMTKN55 to calibrate new hybrid and, in collaboration with Golokesh Santra and Jan Martin of the Weizmann Institute, new double hybrid density functionals as well. Our hybrid and double hybrids are the

best performers in their class reported to date on the GMTKN55 data.
[1] L. Goerigk, et. al. (2017) Phys. Chem. Chem. Phys. 19, 32184

Advances in Reduced Density Matrix Methods

Viktor Staroverov *Western University, ON, Canada.*

We show how to construct analytically all one-electron reduced density matrices compatible with a given electron density within a finite basis set, provided that the density is known as a quadratic from in term of basis functions. Contrary to the current belief, exact linear dependencies in the basis function products assist, rather than hinder, such constructions. Methods for constructing special basis sets required for such density-matrix reconstructions are also presented.

10H15-10H30 | BREAK

10H30-12H00 | CONDENSED MATTER SYSTEMS

Chair: **Richard Bowles** *University of Saskatchewan, SK, Canada.*
Room: D406

Band-by-band chemical shielding contributions

Josef Zwanziger *Dalhousie University, NS, Canada.*

We describe our recently published first-principles method for NMR shielding calculations in solids. We then use it to discuss the origins of the anomalous shieldings observed in 3-5 semiconductors, and along the way test some of the approximations used in this and related approaches to shielding calculations.

Unusual Chemistry and New States of Matter at Extreme Pressure

Eva Zurek *University of Buffalo & SUNY, NY, USA.*

High pressure can be used to access new stoichiometries, crystal structures, and novel electronic and magnetic states of matter that cannot be found at 1 atm. In this talk we present the results of recent first-principles calculations on high-pressure quantum materials that can be formed within diamond anvil cells including electride phases of sodium with unique electronic structures, hydride-based high temperature conventional superconductors, and computational techniques and algorithms that can be used to predict these phases.

Taking precise hybrid DFT simulations of large, complex solids beyond a few old limits

Volker Blum *Duke University, NC, USA.*

This presentation reviews some recent advances in the FHI-aims code and its software ecosystem for efficient, precise all-electron electronic structure simulations of large and complex systems. Within this framework, numeric atom-centered orbital basis sets enable semilocal and hybrid density functional simulations of high accuracy for molecules and periodic solids across the periodic table and from laptops to supercomputers. A series of optimizations is presented that enables hybrid density functional theory calculations well beyond 10,000 atoms in benchmarks, as well as production simulations of several thousand atoms of large complex novel semiconductors. For crystalline hybrid organic-inorganic perovskites, which combine heavy-element based inorganic structure building blocks with complex organic molecules, subtle secondary-bonding interactions shape both the atomic and the electronic structure. Chiral molecules can be inserted to break the inversion symmetry of the inorganic sublattice, leading to spin-dependent carrier properties as a result of relativistic spin-orbit splitting. Supercell calculations well beyond 1,000 atoms enable the prediction of electronic doping levels and their structural origin by direct, spin-orbit coupled hybrid DFT. Overall, the updated implementation enables a wide range of affordable, numerically precise and physically accurate simulations of organic, inorganic and organic-inorganic systems and a host of associated properties in chemistry and materials science.

12h00-13h30 | Lunch

13h30-14h30 | Machine Learning Approaches

Chair: **Jason Pearson** *University of Prince Edward Island, PE, Canada.*
Room: D406

Machine learning force field for inorganic ion conductors

Oleksander Voznyy *University of Toronto, ON, Canada.*

Considering the increasing computational demand posed by ab initio MD simulations, our study addresses the critical need for efficient and accurate MLFFs that can be generated with sustainable use of computational resources. Key highlights of our study include:

- A detailed comparison of state-of-the-art GNN models focusing on their efficiency and accuracy in replicating MD simulations, specifically, for superionic conductors.
- A universal simulation package designed to simplify and integrate various GNN models for energy and force prediction tasks, alongside MD calculations.
- Rigorous tests and demonstration of transferability of the developed MLFFs to unseen materials, showcasing their potential for the discovery of new ionic conductors.
- Proposal of new metrics, beyond conventional accuracy on forces and energies, namely, radial distribution function, diffusion trajectories, and explicit measurement of ionic conductivity. Our findings pave the way for more accessible and efficient molecular dynamics that will enable materials screening based on physics-aware metrics rather than a single-shot output from a machine learning model, incapable of capturing all the subtle details of ionic movement.

Machine learning meets computational chemistry

Rodrigo Vargas-Hernández *McMaster University, ON, Canada.*

Machine learning tools offer significant advantages in computational chemistry, providing innovative approaches to longstanding challenges. This talk will explore several pivotal technologies, starting with automatic differentiation. This technique enhances the accuracy and efficiency of gradient calculations, crucial for molecular inverse design and swiftly tuning semi-empirical models. Additionally, I will discuss the integration of generative models, specifically normalizing flows, with advanced variational inference methods. These are employed as novel ansatzes for solving the electron density problem in orbital-free density functional theory Machine learning tools offer significant advantages in computational chemistry, providing innovative approaches to longstanding challenges. This talk will explore several pivotal technologies, starting with automatic differentiation. This technique enhances the accuracy and efficiency of gradient calculations, crucial for molecular inverse design and swiftly tuning semi-empirical models. Additionally, I will discuss the integration of generative models, specifically normalizing flows, with advanced variational inference methods. These are employed as novel ansatzes for solving the electron density problem in orbital-free density functional theory.

14H30-15H00 | CONTRIBUTED TALKS

Chair: **Jason Pearson** *University of Prince Edward Island, PE, Canada.*
Room: D406

Adaptive hybrid density functionals

Alastair Price *University of Toronto, ON, Canada.*

Exact exchange contributions are known to crucially affect electronic states, which in turn govern covalent bond formation and breaking in chemical species. Empirically averaging the exact exchange admixture over compositional degrees of freedom, hybrid density functional approximations have been widely successful, yet have fallen short to reach high level quantum chemistry accuracy, primarily due to delocalization errors. We propose to 'adaptify' hybrid functionals by generating optimal admixture ratios of exact exchange on the fly, i.e. specifically for any chemical compound, using extremely data efficient quantum machine learning models that carry negligible overhead. The adaptive Perdew-Burke-Ernzerhof based hybrid density functional (aPBE0) is shown to yield atomization energies with sufficient accuracy to effectively cure the infamous spin gap problem in open shell systems, such as carbenes. aPBE0 further improves energetics, electron densities, and HOMO-LUMO gaps in organic molecules drawn from the QM9 and QM7b data set. Obtained with aPBE0 in a large basis, we present a revision of the entire QM9 data set (revQM9) containing more accurate quantum properties with on average, stronger covalent binding, larger band-gaps, more localized electron densities, and larger dipole-moments. While aPBE0 is applicable in the equilibrium regime, outstanding limitations include covalent bond dissociation when going beyond the Coulson-Fisher point.

Interpretability of graph neural networks of chemistry

Amer El-Samman *University of New Brunswick, NB, Canada.*

In recent years, there has been a rise in the use of graph neural network (GNN) machine learning models in chemistry. These are models that fit a relationship between molecular shape and properties by training on data. However, due to the overparametrized nature of these methods, they suffer from a lack of transparency in the decision-making and internal structure. In our work, we delve into a rigorous analysis of a GNN model's internal structure by examining neural network activations in response to molecular input, a.k.a embedding vectors. The embedding vector is a set of activations of the nodal features of an atom-in-a-molecule learned through the GNN training. The embeddings reveal an intricate chemical-based organization of the model's decision-making that can be elucidated in numerous ways. Firstly, the embeddings cluster visibly and quantitatively in regions representing functional groups of the trained database. Moreover, these clusters adhere to a Euclidean distance measure of molecular similarity. Most interestingly, the embedding vector space displays a linear algebraic analogy to chemical reaction syntax. By adding and subtracting embedding vectors, we show that the embedding space models reaction formulas in a self-consistent manner. Lastly, we show that the embedding vector space contains enough information to guide the training on new properties (pKa, NMR, and solubility) with very little data. This work explores a much-needed interpretation of modern statistical techniques as the AI revolution takes hold of the chemical sciences.

15h00-15h15 | Break

15h15-16h00 | Contributed Talks

Chair: **Gilles Peslherbe** *Concordia University, QC, Canada*
Room: D406

A New Framework for Protein Allostery Predictions Based on Incomplete NMR Data

Fanwang Meng *Queen's University, ON, Canada. McMaster University, ON, Canada. Massachusetts Institute of Technology, MA, USA.*

Deciphering protein allostery is important for understanding cellular regulation and inspiring strategies for drug design. Therefore, numerous efforts have been dedicated to identifying allosteric sites and mapping allostery networks, both experimentally and computationally. A promising strategy is to use robust and reliable experimental biophysical data to predict protein allostery. In particular, Nuclear Magnetic Resonance (NMR) is a powerful tool for probing protein dynamics and elucidating the structural basis of allostery at atomic resolution. However, when measurements for selected residues are missing, predicting allostery becomes more challenging. Here, we address this gap by proposing a new computational model for protein allostery prediction using sparse NMR data. This new framework enables to predict which amino acid residues are in the allostery network, even when not all of the relevant residues' chemical shifts can be measured. More specifically, the matrix completion, a recommender system algorithm, is used to impute missing NMR data. A numerical experiment is also performed to assess the performance of the matrix completion for recapitulating the missing NMR data. Then an unsupervised machine learning algorithm, robust independent component analysis, is employed to map protein allostery. This computational framework is used to map protein allostery of the Exchange Protein directly Activated by cAMP (EPAC), a promising drug target. We show that through the proposed method several previously missing and allosterically important EPAC residues are now identified in agreement with independent experimental validations.

Quantum Correlation in Dipeptide Systems: A Quantum Information Theoretic Approach

Mostafa Javaheri Moghadam *University of New Brunswick, NB, Canada*

Proteins are large and complex biomolecules that perform a range of biological functions. To understand the complexities of proteins structure and functionality, it is crucial to study the chemical interactions of their building blocks, amino acids. Proteins are made up of 20 naturally occurring amino acids that links together in various combination and forms the primary structure of proteins which in turn determines its tertiary functional structure. While high-quality ab initio methods are required for capturing an accurate description of amino acids' interactions, these methods are only applicable to medium-sized systems. As a result, using less advanced techniques like force fields and molecular dynamic simulations is the only way to explore larger systems. Nevertheless, the accuracy of these methods is inferior compared to ab-initio methods as they don't account for quantum correlation energy contribution. In our study, we applied the concept of quantum mutual information to understand the chemical interactions of amino acids. Our analysis focused on the entanglement between pairs of atomic orbitals embedded in the environment of all other active-space orbitals. Using von Neumann entropy and a one- or two-particle reduced density matrix, we evaluated the orbital entropy and the atomic mutual information for a variety of dipeptides. Our results show that the atomic mutual information provides a useful tool for measuring the strength and character of chemical bonding in biomolecules. By investigating these metrics, we can uncover potential interactions between amino acids and broaden their applicability to larger systems.

Accounting for the Electrode Potential in Modeling Processes at the Solid-Electrolyte Interface with Grand Canonical Ensemble DFT: The Potential-Dependent Competition of NRR and HER

Mehdi Shamekhi *Concordia University, QC, Canada.*

Electrochemical reactions take place at the solid-electrolyte interface, however, modeling of these processes at the atomic scale is challenging and may require techniques beyond conventional models. The standard quantum chemistry approach to model proton-coupled electron transfer steps in electrochemical reactions is the computational hydrogen electrode, a limitation of which lies in the neglect of the potential experienced by the electrode material. On the other hand, grand canonical ensemble density-functional theory (GC-DFT) allows the treatment of a system at fixed electrode potential by fixing the Fermi level and varying the number of electrons in the simulation box. Accordingly, we evaluate adsorption energies of intermediates and activation energies of selected electrochemical reactions at constant electrode potential and compare with the results of standard methods to assess the influence of maintaining a constant electrode potential in the simulations. As a case study, we characterize the potential limiting step of the nitrogen reduction reaction (NRR) and the hydrogen evolution reaction (HER) on transition metal surfaces via GC-DFT. The HER is found to be more favourable than the NRR with increase in the electrode potential, a feature that is not predicted by standard DFT, and rationalizes the premature decrease in NRR activity observed experimentally. This highlights the importance of accounting for the electrode potential in computational investigations of the thermodynamics and kinetics of electrochemical reactions.

Molecular Dynamics Simulations of Thermal Transport in Single-Molecule Junctions

Jonathan Wang *University of Toronto, ON, Canada.*

With the objective of understanding microscopic principles governing thermal energy flow in nanojunctions, we study phononic heat transport through metal-molecule-metal junctions using classical molecular dynamics (MD) simulations. Considering a single-molecule gold-alkanedithiol-gold junction, we first focus on aspects of method development and compare techniques for calculating thermal conductance: (i) Langevin Nonequilibrium MD (LNEMD) method, which generates nonequilibrium steady state with Langevin thermostats at boundaries of the junction. (ii) Reverse Nonequilibrium MD (RNEMD) method, where heat is inputted and extracted at a constant rate from opposite metals to form a temperature bias at steady state. (iii) Approach-to-Equilibrium MD (AEMD) method, with the thermal conductance of the junction obtained from the equilibration dynamics of the metals. Simulations of the same junction with all methods show consistent magnitudes of thermal conductance, and chains of a growing size display an approximate length-independence of the thermal conductance, with calculated values matching computational and experimental studies. In addition, heat exchange statistics was examined for method (i), where it was shown that while the average heat current across the junction behaves physically, the probability distribution of the current violates fundamental fluctuation symmetry. We then apply our methods by (1) characterizing gold-buckminsterfullerene-gold junctions to investigate thermal transport behavior of stacking fullerenes and (2) attempting to induce thermal diode effect by introducing asymmetry in the gold-alkanedithiol-gold junction. Both applications advance knowledge towards achieving phonon control and designing nanoscale devices, such as thermoelectrics and nonlinear thermal devices.

Utilizing the Max-Cut Problem in Quantum Circuit Design to Simulate Ground States of Spin Glasses

Ehsan Ghasempouri *University of New Brunswick, NB, Canada.*

Exploring the ground-state properties of Ising spin glasses stands as a significant challenge in both solid-state physics and statistical mechanics. The term ”Ising spin glass” denotes a state of disordered magnetism where the spins of magnetic atoms or molecules interact, resulting in intricate and frustrated magnetic phenomena. The behavior of frustrated magnetic metals is observed in alloys such as CuMn and AuFe, where manganese (Mn) or iron (Fe) is introduced as impurities into copper (Cu) or gold (Au). The Ising model is widely employed due to its simplicity and accuracy in representing real-world phenomena, as it can effectively model actual systems on a lattice. The presence of unsatisfied edges in the lattice can lead to situations where multiple geometric arrangements of atoms remain stable. Consequently, the system may exhibit various forms of resonance, complicating the consideration of interactions between magnetic sites. In this study, our objective is to simulate a frustrated system consisting of a triangular spin-lattice up to 10 sites. To construct an efficient circuit that effectively links various qubits, we organize them into separate clusters within the quantum circuit. This is achieved by employing the maximum cut technique, which involves dividing the lattice into two distinct groups and establishing connections between them. We utilize the Variational Quantum Eigensolver (VQE) method to compute the energy.

19H00-21H00 | BANQUET

Day 3: Wednesday July 24

09H00-10H15 | CATC LECTURE

Chair: **Tom Woo** *University of Ottawa, ON, Canada.*
Room: D406

Uncovering the Inner Lives of Electrons

Paul Ayers —CATC Medal— *McMaster University, ON, Canada.*

The chemical reactivity and physical properties of molecules are determined by the behavior of their electrons, which makes it essential for us to understand how, and on a more philosophical level, why, electrons behave as they do in different environments. I’ll present some of our new work on modelling molecules’ electronic structure, especially when the electrons are strongly correlated. Specifically, I’ll discuss new wavefunction forms that provide a more faithful representation of molecular electronic structure, and discuss how they can be supported through the FANCI (flexible ansatze for N-electron configuration interaction) framework and its extensions to perturbation theory (FANPT) and response/spectroscopic properties (FANEOM). I’ll conclude with some thoughts on how one can use quantum-mechanical observables to elucidate molecular electronic structure and chemical reactivity.

Insight into flat-plane conditions from spin-constrained Full CI wavefunctions.

Patrick Bultinck *Ghent University, Belgium.*

The failure of many approximate electronic structure methods can be traced to their erroneous description of fractional charge and spin redistributions in the asymptotic limit toward infinity, where violations of the flat-plane conditions lead to delocalization and static correlation errors. However, such errors can only be characterized sufficiently in terms of those redistributions if exact energies are available for many possible (spin)population redistributions at different bonding distances. We propose to model such redistributions by imposing (spin)populations on atomic domains by constraining full configuration interaction wave functions. The resulting N-representable descriptions of small hydrogen chains at different bonding distances allow us to computationally illustrate the effects of the flat-plane conditions in the limit to infinite bond distances, leading to more chemical insight into those flat-plane conditions.

10h15-10h30 | Break

10h30-12h00 | Wavefunction Theory

Chair: **Farnaz Heidar-Zadeh** *Queen's University, ON, Canada.*
Room: D406

Single Reference Treatment of Strong Correlation with Richardson-Gaudin States

Paul Johnson *Université Laval, QC, Canada.*

Weakly-correlated systems are well described as individual electrons. The dominant contribution to the wave function is a Slater determinant of the occupied orbitals, with small corrections from single- and double-excitations. This is not the case for strongly-correlated systems. Many Slater determinants contribute substantially and thus the correct physical picture is not independent electrons. For molecular systems, we have shown that Richardson-Gaudin (RG) states are a much better starting point. They amount to pair wave functions, but they are tractable and form a basis of the Hilbert space, allowing for systematic improvement. Simple corrections are shown to account for the remaining weak correlation.

Converging High-Level Coupled-Cluster Energetics via Semi-Stochastic, Selected-CI-Driven, and Adaptive CC(P;Q) Approaches

Piotr Piecuch *Michigan State University, MI, USA.*

It is well established that the exponential wave function ansatz of coupled-cluster (CC) theory and its extensions to excited, open-shell, and multireference states are among the most efficient ways of incorporating many-electron correlation effects in molecular applications. In this talk, we will discuss novel ways of obtaining accurate energetics equivalent to high-level CC and equation-of-motion (EOM) CC calculations, such as CCSDT, CCSDTQ, and EOMCCSDT, at small fractions of the computational costs, even when electronic quasi-degeneracies become large and higher–than–two-body components of the relevant cluster and excitation operators become nonperturbative, which result from merging the moment expansions that define the CC(P;Q) framework with Quantum Monte Carlo (QMC) propagations in the many-electron Hilbert space and with the selected configuration interaction (CI) approach abbreviated as CIPSI. We will conclude by highlighting an adaptive, self-improving, CC(P;Q) formalism, which frees us from the originally exploited active orbitals and the more recently utilized non-CC (CIQMC, CIPSI) or stochastic (CIQMC, CCMC) concepts by taking advantage of the intrinsic mathematical structure of the CC(P;Q) moment expansions in defining the underlying excitation manifolds. The usefulness of the semi-stochastic, CIPSI-driven, and adaptive CC(P;Q) methodologies will be illustrated by chemical bond dissociations and reaction pathways, singlet–triplet gaps in biradicals, and excited states including one- as well as many-electron transitions. Information about the availability of CC(P;Q) methods in the GAMESS and CCpy packages will be provided as well.

Developments in Nonorthogonal Multiconfigurational Self-Consistent Field Theory and Applications to Modeling Nonadiabatic Processes

Lee Thompson *University of Louiville, KY, USA.*

Nonorthogonal multiconfigurational self-consistent field (NOMCSCF) theory describes the wave function in terms of a 'different orbitals for different configurations' expansion. The advantage of such an approach is that 1) each determinant is described using the best set of orbitals for a given electron configuration, and so static and differential dynamic correlation can be recovered, 2) the NOMCSCF approach can be used to reveal correlation mechanisms within the wave function that indicate partitioning of strong correlation, and 3) the NOMCSCF adiabatic states can be obtained in terms of a quasidiabatic determinant basis. However, there are a number of challenges remaining in order to develop the method to allow it to tackle problems of chemical interest. In this presentation I will describe recent work from my group to develop robust wave function optimization methods, explore the role of spin and spatial symmetry in providing a description of correlation mechanisms, and how such an approach has been applied to study of energy transfer mechanisms.

12H00-13H30 | LUNCH

13H30-14H30 | QUANTUM COMPUTING

Chair: **Thomas Baker** *University of Victoria, BC, Canada.*
Room: D406

Open quantum systems and current quantum computation

Kade Head-Marsden *University of Minnesota, MN, USA.*

Dissipative quantum dynamics are ubiquitous in nature yet challenging to theoretically predict. Recent progress in quantum algorithms has allowed for the prediction of non-unitary time dynamics of quantum systems using current Noisy-Intermediate Scale Quantum computers. While this field continues to progress, there is an on-going search for alternative platforms for quantum computation, and molecular qubits have arisen as a possibility. The candidacy of a molecular qubit will depend on the coherence time of an electronic state, a property that will depend heavily on interactions with a complex environment. Here, I will discuss the interplay between current quantum computation and methods from the study of open quantum systems.

Improved Hamiltonian pre-processing for Quantum Computing

Matthias Degroote *Boehringer-Ingelheim, The Netherlands.*

The quantum phase estimation algorithm stands as the primary method for determining the ground state energy of a molecular electronic Hamiltonian on a quantum computer. Current run time estimates are still too long to be practical. In this talk I will present an improvement in the decomposition of the Hamiltonian and in the overlap of the initial state with the final wave function. Both techniques use classical quantum chemistry techniques to reduce the cost of quantum simulation, showing the importance of choosing the right representation in order to achieve the best computational efficiency.

Quantum Circuits for the Electronic Structure Problem

Jakob Kottmann *University of Augsburg, Germany*

I will present some novel approaches that leverages unitary coupled-cluster (UCC) principles tailored for quantum computers. We will see an introduction to the underlying design principles for such bottom-up approaches, allowing exploration of multiple orbital bases and cost-effective introduction of correlations. Unlike traditional coupled-clusters, the methodology allows operations in multiple orbital bases. A key guiding heuristics into the grouping and initialization of the orbital bases is provided by valence bond resonance structures. We explicitly demonstrate initial methodologies on several benchmark systems highlighting the advantages compared to standard UCC approaches and local bottom-up approaches.

15h00-15h15 | Break

15h15-16h00 | CATC Meeting

All independent researchers based in Canada are invited to attend the CATC Meeting
Room: D406

19h00-21h00 | Poster Session

Room: Sexton Memorial Gym, Building J
Abstracts: See Poster Abstracts on page 24

Day 4: Thursday July 25

09h00-10h15 | Biochemistry

Chair: **Heather Wiebe** *Vancouver Island University, BC, Canada.*
Room: D406

In silico hit discovery from ultra-large chemical libraries

Francesco Gentile *University of Ottawa, ON, Canada*

It has been estimated that the drug-like chemical space of small molecules contains more than 1060 molecules. Recent efforts to access such space have led to the development of virtual make-on-demand libraries consisting of billions of synthesizable molecules, paving the way for new opportunities in drug discovery. To deal with these enormous databases, AI-accelerated virtual screening methods have rapidly emerged as leading strategies for hit identification in early-stage drug discovery, both in academia and industry. One such method developed by us is Deep Docking, which combines computational docking with machine learning to rapidly identify the most promising molecules in a library based on their 2D chemical structures. This is achieved by training a model with the docking scores of just a small fraction of the library, then iterating the process through an active learning cycle. In this talk, we will highlight recent advancements introduced in the Deep Docking platform, and we will present a series of successful case studies of ultra-large virtual screening against clinically relevant targets that led to the identification of novel scaffolds. Taken together, these results highlight the increasing role of machine learning techniques coupled with physics-based methods to streamline chemical discovery for drug targets on a large scale.

Computational Insights Into New and Novel –S–N– and –S–O–N– Peptide and Protein Crosslinks

James Gauld *University of Windsor, ON, Canada*

Thiols, sulfides, and amines are ubiquitous functional groups in cells and organisms. Individually, they are critical for many physiologically important reactions and species. For instance, many enzymes contain a catalytic cysteinyl that acts as an acid/base or nucleophile. It has long been recognized that under relatively mild conditions thiols and amines react with each other to form –S–N– bonds. However, to date, only $\sim$ 100 –S–N– containing biomolecules have been identified. Recently, experimental studies have suggested the reversible redox formation of an –S–O–N– crosslink between the thiol and amine side chains of an active site cysteinyl and lysyl in a transaldolase enzyme. It is proposed to play an important role in regulation of the enzymes function. In addition, it has also been proposed that such -S-O-N- reversible redox crosslinks, or switches, are possibly widespread in proteins. Indeed, a redox-induced –S–O–N(R)–O–S– crosslink involving two cysteines and a lysine has been observed in the main protease of SARS-CoV-2. Despite these experimentally observed occurrences, much remains unknown about such crosslinks including their nature and properties, and how they may be formed within proteins/enzymes. Our research group employs multi-scale computational approaches to the elucidate the nature and possible formation of –S–N– and –S–O–N– crosslinks in enzymology as well as for the formation of new peptides. In this presentation, some recent results and insights from our studies will be highlighted.

10h15-10h30 | Break

10h30-12h00 | Solid State Physics & Chemistry

Chair: **Leanne Chen** *University of Guelph, ON, Canada.*
Room: D406

Reaction Modelling in Catalytic Atomic Layer Deposition

Irina Paci *University of Victoria, BC, Canada*

Atomic layer deposition (ALD) is a self-limiting, cyclic gas phase deposition technique used to grow highly conformal layers of an inorganic material. ALD is becoming the deposition method of choice for the fabrication of complex semiconductor materials and microelectronic devices because it offers new possibilities for advanced nanopatterning through selective deposition and deposition onto high aspect ratio substrates. Despite its growing popularity, ALD mechanisms remain poorly understood and only a handfull of reaction pathways are known, yet rational design of new precursors for ALD is desirable to optimize layer conformity, selective deposition and reaction conditions for a broad variety of materials. One such process is the selective deposition of cobalt on a variety of substrates, a target with important applications in microelectronics. In this presentation, I will focus on our group's efforts to examine the catalytic deposition mechanisms of current and newly designed Co and SiO_2 precursors on metallic substrates, Si and SiO_2.

Modern Challenges in Organic Crystal Structure Prediction

Gregory Beran *University of California Riverside, CA, USA*

Molecular crystal structure prediction has been transformed in recent years, thanks in large part to advances in dispersion-corrected density functional theory (DFT). Crystal structure prediction is increasingly used in the pharmaceutical industry to help de-risk solid-form selection for new drugs. Nevertheless, there remain significant challenges, two of which will be discussed here. First, despite many successes, the density functionals often used to model the solid state, especially generalized gradient approximation (GGA) functionals, suffer from delocalization error effects that can lead to highly erroneous relative lattice energies in certain systems. We will discuss examples of this behaviour, including two contrasting examples from the recent 7th Blind Test of Crystal Structure Prediction, and will present our solution for addressing these issues. Second, while many crystal structure prediction efforts have focused on predicting the structures and their physical properties, few have sought to predict the solid-state chemical reactions or have considered how to design organic materials with desirable chemical reactivity. We will present recent work toward understanding and designing improved photomechanical crystals in light is converted to mechanical work through solid-state organic photochemical reactions.

Deriving phase field crystal theory from dynamical density functional theory: Application to microstructure evolution

Conrard Tetsassi Feugmo *University of Waterloo, ON, Canada*

Conventional modelling methodologies, such as first principle density functional theory and classical molecular dynamics, can explore atomic length scales but are limited by their computational costs when examining beyond the order of nanoseconds. Phase field crystal (PFC) modelling is a recent simulation methodology that overcomes this limitation by accessing atomic length and diffusive time scales, making it a credible and computationally efficient alternative to conventional approaches [1]. The earliest variant of the PFC model incorporated a free-energy functional inspired by the Swift-Hohenberg equation, which was minimized for periodic crystalline lattices with required symmetry. This approach naturally incorporated elastic and plastic deformation in crystalline systems while accessing diffusive time scales. It was later shown that the PFC model based on the Swift-Hohenberg equation could be derived from the theory of classical density functional theory of freezing (cDFT) [2], demonstrating its theoretical foundations. Since then, several variants of PFC have emerged, including amplitude expansion PFC (APFC), structural PFC (XPFC), vapour PFC (VPFC), and hydrodynamic PFC (HPFC), highlighting its promising future for computational materials research. This study focuses on developing and applying the structural (XPFC) variant of the PFC model for high entropy alloy applications. The XPFC approach modifies the free energy functional by introducing multi-peak two-point direct correlation functions expressed by a Gaussian function in reciprocal space. The current work aims to simulate high entropy alloys characterized by highly disordered microstructures and lattice frustration due to their multiple components. The model evolves the system's atomic density fields over time using spectral techniques and fast Fourier transform algorithms.

[1] H. Emmerich, et. al. (2012) Adv. Phys. 61, 665.
[2] K. R. Elder, et. al. (2017) Phys. Rev. B75, 064107.

12H00-13H30 | LUNCH

13H30-14H30 | LIGHT-MATTER INTERACTIONS

Chair: **Michael Schuurman** *National Research Council, ON, Canada.*
Room: D406

Chemical bonding and Molecular Properties

Jochen Autschbach *University of Buffalo, NY, USA*

How does chemical bonding impact molecular properties? We can learn about the underlying relationships via quantum theoretical calculations. This talk will survery selected recent studies focusing on electronic structure - chemical bonding - molecular properties relationships in a range of areas, including properties of transition metal, lanthanide, and actinide complexes as well as other types of compounds with closed and open shells. Selected topics will include core-shell excitations in f-element complexes, and the use of density-corrected DFT to calculate molecular properties. If time permits, I will also discuss the curious electronic structure of certain radials that have been assigned by some as having non-aufbau ground state configurations.

Data-driven discovery of molecules with unique excited states for next-generation organic electronics

Terrence Blaskovits *Max Planck Institute for Polymer Research, Germany*

A bottleneck in the application of machine learning (ML) to organic electronic materials is the lack of relevant data. In fact, most developments in ML for chemistry have focused on few datasets and on ground state properties. While large in size, these datasets lack the compositional complexity and diversity representative of the chemical space required for the design of new materials with tailored optoelectronic properties. Furthermore, existing datasets may contain chemically unrealistic compounds.

To address these challenges, we developed a dataset of over 110K experimentally-reported organic molecules, curated from a crystal structure repository, as well as protocols to automate the coupling of these molecules together in chemically meaningful ways.[1] The dataset size and chemical diversity enable the training of gradient boosting models for the prediction of excited state energies with excellent accuracy across experimental compound space. These models enable on-the-fly evaluation of excited states in the screening of a million potential candidates for singlet fission (SF) - a multiexciton-generating process that is a promising route to increased solar cell efficiencies through the conversion of one excited singlet state into two triplet states.

The models and dataset are then redeployed in the multiobjective genetic optimization of SF candidates.[2] We show that calibrated prediction uncertainty can be used to guide the algorithm towards low- or high-uncertainty regions of chemical space. In the former (‘exploitative’) setup, variations of known SF compounds are uncovered. In the latter (‘explorative’) mode, altogether new yet synthetically feasible candidates are generated which display excellent electronic properties for SF.

[1] J. T. Blaskovits, et. al. (2024) Adv. Mater. 36, 2305602.
[2] L. Schaufelberger, et. al. (2024), Manuscript in preparation.

Non-Adiabatic Spectroscopy and Dynamics: The Linear Vibronic Coupling Model and Beyond.

Graham Worth *University College London, UK*

The Linear Vibronic Coupling (LVC) Hamiltonian is a standard model used to describe a manifold of coupled electronic states. It has been used with great success to simulate the absorption spectrum and underlying nuclear dynamics of a number of problems. On top of its simple descriptive power, one of its strengths lies in its mathematical form that allows it to be used for accurate solutions of the time-dependent Schrödinger equation (TDSE). However, while it is well suited for describing short-time dynamics, it is not able to treat long-range motion, such as found in photochemical change. For this reason, it is sometimes necessary to go to higher order potentials, or to find other strategies to solve the TDSE. In this presentation, examples of calculations beyond the simple LVC model will be presented. These include the photo-excited dynamics of maleimide and thiophene, along with the photoionisation dynamics of cyclobutadiene.

15H00-15H15 | CLOSING

Poster Abstracts

P01 | Properties and construction of linearly independent product basis sets

Georgii Sizov *Western University, ON, Canada*

Linearly independent product (LIP) basis sets have remarkable applications in quantum chemistry but are uncommon. We establish certain mathematical properties of LIP basis sets which facilitate their construction. The findings are illustrated with examples.

P02 | DMRjulia v1.0

Thomas Baker *University of Victoria, BC, Canada*

I discuss the v1.0 debut of the entanglement renormalization software, DMRjulia. The library is written for the Julia programming language and has been used in several papers to discover new solutions of quantum materials and simulate quantum algorithms. I discuss how to use this library for practical computation in both physics and chemistry, including tensor-graph ansatzs that are easily produced in the library (MPS, PEPS, MERA), and future directions of the library

P03 | The Fermi-Amaldi Functional for Fractional Densities

Ivan Bosko *Western University, ON, Canada*

The Fermi-Amaldi density functional is an exact exchange-energy functional for systems with one occupied orbital or with any number of equally populated orbitals that have zero differential overlap. We discuss various challenges and ways of generalizing this functional to systems with a fractional number of electrons.

P04 | Are exchange-correlation potentials discontinuous at atomic nuclei?

Conrad Moore *Western University, ON, Canada*

Kinetic energy densities are known to be discontinuous at the atomic nuclei in molecules, which through certain exact relations implies that exact exchange-correlation (XC) potentials might be discontinuous there as well. This is made even more likely by the fact that XC potentials are certainly discontinuous at the nuclei within Slater-type basis sets. We show that, in the basis-set limit, all actual discontinuities cancel out exactly but nontrivially.

P05 | Interactions in a Coarse-Grain Scheme for Liquids

Mark Thachuk *University of British Columbia, BC, Canada*

Using a previously-developed coarse-grain (CG) scheme for liquids, the interactions among CG blobs will be described. These effectively take the form of a generalized quadratic function with parameters depending upon the location of nearest neighbour blobs. We also show how these parameters can be evaluated from the atomistic pair distribution function using expressions derived from a statistical mechanical description. The behaviour of the system as a function of the fuzziness of the boundaries between blobs is also explored, including in the thermodynamic limit.

P06 | Macroscopic behaviour of the dimer model

Veronika Keras *Dalhousie University, NS, Canada*

The dimer model is a mathematical model that describes the placement of dimers on a grid. Mathematically this corresponds to a domino tiling. It has been observed by Cohn et. al. [1] that the qualitative behaviour of random domino tilings is very sensitive to the shape of the region's boundary and can be described by the solution to a certain partial differential equation that can be derived from a variational principle. Depending on the shape of the boundary, they may also exhibit macroscopic behaviours such as phase transitions. In this poster, I will report on the results of my summer research on the combinatorics of macroscopic behaviour of the dimer model.

[1] H. Cohn, R. Kenyon & J. Propp. (2011) J. Amer. Math. Soc. 14, 297.

P07 | Pair Approximating The Action For Molecular Rotations

Shaeer Moeed *University of Waterloo, ON, Canada*

Path integral Monte Carlo (PIMC) studies are ubiquitous in theoretical chemistry and condensed matter physics. Typical approaches use the primitive approximation to compute the probability density for a given path. In this work, we propose employing the pair approximation instead for studying molecular rotations. The pair propagator was initially introduced to study superfluidity in Helium since it reduces the root-mean-square error by a factor of 20 compared to the primitive approximation. Moreover, the form of this propagator is a product of two-body terms which is naturally well-suited for systems interacting with a pair-wise potential. Consequently, paths sampled using the pair action tend to be closer to the exact action (compared to primitive) leading to convergence with a smaller number of beads. In this work, we use the pair propagator in conjunction with a discretized PIMC paradigm to study a chain of planar rotors interacting with a pair-wise dipole interaction. Leveraging the better convergence properties of the pair approximation allows us to circumvent the sign problem and probe the thermodynamic limit required for studying interesting statistical phenomena such as quantum phase transitions (QPTs). To this end, we first exhibit the utility of the pair propagator for this system via convergence studies comparing the primitive and the pair approximations. Then, we compute energetic and structural properties for $N = 100$ such as the chemical potential, correlation function and Binder ratio to examine the QPT in this system. Density Matrix Renormalization Group results are used for benchmarking throughout.

P08 | Many-body potential energy surfaces for parahydrogen, and simulations of solid parahydrogen

Alexander Ibrahim *University of Waterloo, ON, Canada*

The topic of many-body interactions has seen a rise in interest over the past few decades, and the relative simplicity of hydrogen makes it an excellent research subject. Solid parahydrogen is a quantum molecular solid below 13.8 K, and displays many exotic properties not seen in classical solids. One of the most significant of these properties is the large zero-point kinetic energy of the parahydrogen molecules, allowing them to move about their nominal lattice sites near absolute zero. This large zero-point motion allows the parahydrogen molecules to interact at distances much shorter than the lattice constant. This close proximity causes many-body interactions to be relevant in solid parahydrogen even at relatively low densities. Two-body interaction potential energy surfaces (PES) on their own are inherently insufficient for accurately modelling or simulating solid parahydrogen. An accurate description of solid parahydrogen requires higher-order many-body PESs. A few years ago, our group created an ab initio three-body PES for parahydrogen clusters, and performed path-integral Monte Carlo (PIMC) simulations of solid parahydrogen using both two-body and three-body PESs. The three-body PES improved agreement between simulation and experiment at low densities, but was insufficient at higher densities. Recently, our group created a neural network-based ab initio four-body PES for parahydrogen clusters. Its inclusion alongside the two-body and three-body PESs in PIMC simulations of solid parahydrogen is expected to improve the agreement between simulation and experiment to higher densities.

P09 | The QC-Devs Software Ecosystem

Farnaz Heidar-Zadeh *Queen's University, ON, Canada*

QC-Devs (qcdevs.org) is an international software community devoted to developing sustainable software for quantum chemistry, physics, and the computational sciences. Our goal is to make programming accessible to researchers, to catalyze scientific collaboration, and to promote precepts of sustainable software development. Towards this end, we are actively developing free, open-source, and cross-platform libraries for scientific computing, focusing on theoretical and computational chemistry. We're adapting some of the same principles to develop free and open-source educational materials (qchem.qc-edu.org). The goal of this presentation is to familiarize the audience with the current QC-Devs software landscape and philosophy. We'll discuss the (sometimes painful) lessons we've learned along the way, and describe how we've arrived at our current (yet constantly evolving) software development principles and protocols. In addition, we'll discuss the future development of QC-Devs and encourage others to join the team.

P10 | Machine learning seams of conical intersection: A characteristic polynomial approach

Joey Wang *University of Ottawa, ON, Canada*

Machine learning of potential energy surfaces (PES) has seen rapid progresses in recent years, the majority of which focuses on the learning of ground state PES. Difficulties arise in the direct learning of adiabatic excited surfaces due to the existence of seams of conical intersections, which are discontinuous and renders standard learning methods ineffective. We show that this may be overcome by instead learning the characteristic polynomial coefficients that form a fundamental representation of PES which are smooth and amenable to machine learning

P11 | Neural Network Potentials Using a Matrix-Based Descriptor

Omid Tarkhaneh *Memorial University, NL, Canada*

Molecular properties prediction using machine learning potentials has been a popular research area in computer science and computational chemistry over recent years. To predict properties of molecules, such as total energy, the basic idea is to use features of the molecules such as coordinates (positions) and charges as input into a neural network. One challenge with this approach is that the data should be invariant to rotation, translation, and permutation. In this regard, some types of descriptors, such as the Coulomb matrix, are introduced, which are used to feed the neural networks and perform the prediction. Having a good descriptor has a significant impact on the final results of the neural network model. Using a robust model is also important. In this research, a new model, along with a matrix-based descriptor, is employed to predict the molecular total energy. The proposed model uses the Behler-Parrinello approach using a Multilayer Perceptron Neural Network (MLP). The results show that the proposed descriptor is able to predict the total energy of molecules efficiently using measures such as mean absolute error and root mean squared error.

P12 | New insight into correlated electron motion: relative angular momentum

Josh Hollett *University of Winnipeg, MB, Canada*

Given that the usual reference for electronic structure calculations is that of ”independent” electrons, our understanding is shaped by the one-electron picture. While the picture is qualitatively useful for understanding such things as chemical reactivity, it ignores electron correlation which is responsible for the nuances of electronic structure and quantitatively accurate models. Augmenting our picture to incorporate the relative motion of electron pairs improves our basic understanding of electronic structure, the various classifications of electron correlation and can lead to improved models. Recently we defined momemtum-balance, a measure of the relative momentum of electrons and a signature of potential-dependent correlated motion which is related to the usual ”static” correlation. Our development of models for the remaining electron correlation, so-called ”dynamic”, has revealed the importance of relative angular momentum which is already known to determine the form of the electron-electron cusp. Therefore, we have defined a measure of the relative angular momentum of electrons, as well as a distribution centred at the electron-pair centre-of-mass. An investigation of this measure and distribution, in simple ”toy” systems and chemical systems exhibiting prototypical forms of electron correlation will be discussed along with the incorporation into two-electron-density functionals for the correlation energy.

P13 | Low Thermal Expansion of Layered Electrides Predicted by Density-Functional Theory

Adrian Rumson *Dalhousie University, NS, Canada*

Layered electrides are a unique class of materials with anionic electrons bound in interstitial regions between thin, positively charged atomic layers. While density-functional theory is the tool of choice for computational study of electrides, there has to date been no systematic comparison of density functionals or dispersion corrections for their accurate simulation. There has also been no research into the thermomechanical properties of layered electrides, with computational predictions considering only static lattices. In this work, we investigate the thermomechanical properties of five layered electrides using density-functional theory to evaluate the magnitude of thermal effects on their lattice constant and cell volumes. We also assess the accuracy of five popular dispersion corrections with both planewave and numerical atomic orbital calculations.

P14 | Substituent Properties as Features in Machine Learning Models

Robert Mawhinney *Lakehead University, ON, Canada*

Manipulation of chemical properties via changes in substituents is a well know tool used my chemists. The experimental parameters for describing the effects of such substitutions are based on the approach developed by Hammett that can be readily reduced to an isodesmic reaction involving the substituted and unsubstitiued reaction energies. Anecdotaly, these have been attributed to substituent propeties such as electron donating, electron withdrawing, resonance, and field contributions. Severeal years ago we began compiling substituent specifc properties from the Quantum Theory of Atoms In Molecules, assessing the effects of model chemistry, their transferability between substrates, and relationships to Hammett parameters. Herein, I will discuss recent property updates, including a more robust axis system and incorporation of atomic critical points, and describe their use as features in machine learning models.

P15 | Matching ROY Crystal Structures to High Throughput PXRD

Grace Sparrow *Dalhousie University, NS, Canada*

The ability of a compound to form different crystalline structures is known as polymorphism, where polymorphs will possess different chemical and physical properties. To identify the isolable polymorphs of a compound, extensive experimental screening of crystallization conditions is often carried out in a high-throughput fashion, where only powder X-ray diffractograms (PXRD) are obtainable. To identify if a particular solid form is a new or pre-existing polymorph, the room-temperature PXRD must be compared to low-temperature single crystal X-ray structures, such as from the Cambridge structural database (CSD). This comparison is problematic because the diffractogram peak positions shift substantially with temperature. To address this challenge, the variable-cell experimental powder difference (VC-xPWDF) method was developed and allows for reliable comparison of experimental PXRD to simulated diffractograms of known crystal structures. This work assesses the performance of VC-xPWDF for high-throughput polymorph screening for the test case of 5-Methyl-2-[(2-nitrophenyl)amino]-3-thiophenecarbonitrile, also known as ROY, which is a prolific polymorph former. The method is shown to be successful for comparison of PXRD to both experimental crystal structures from the CSD and computationally generated structures obtained from Beran's previous crystal structure prediction study. The experimental PXRD quality was shown to not affect the results significantly, except for errors occurring due to preferential orientation, which could potentially be reduced by some minimal grinding of the samples prior to making the PXRD measurements. Overall, this work demonstrates the utility of VC-xPWDF to solve crystal structures from PXRD data generated during high-throughput polymorph screening.

P16 | The effect of quasi-one-dimensional confinement on dynamical heterogeneities in glass forming liquids.

Josh Gramlich *University of Saskatchewan, SK, Canada*

Confined fluids display unique characteristics in comparison to bulk fluids. The geometrical constraint of the confining walls introduces incommensurate length scales in particle-particle and particle-wall interactions which lead to fundamental changes in the phase behaviour of glass forming liquids, with either enhancement or suppression of the glass transition [1], T_g, as well as re-entrant crystallization [2] with respect to the degree of confinement. Bulk liquids near the glass transition exhibit dynamical heterogeneities, where local relaxation rates that fluctuate strongly over space and time [3]. Here, we use molecular dynamics to see how confinement to long narrow channels effects dynamical heterogeneities in a 2D binary Kob-Andersen (KA) Lennard-Jones (LJ) mixture as a function of channel diameter. We investigate several dynamic and structural properties including the mean squared displacement, radial distribution function, bond-orientational order parameter and bond-breaking correlation function as the supercooled liquid approaches the glass transition as a function of channel diameter.

[1] T. S. Ingebrigtsen, et. al. (2013) Phys. Rev. Lett. 111, 235901.

[2] J. Mittal, et. al. (2008) Phys. Rev. Lett. 100, 145901.
[3] R. K. Pandit & H. E. Castillo (2023) Phys. Rev. Lett. 131, 218202.

P17 | Fermionic Molecular Dynamics

Vivek Das *University of New Brunswick, NB, Canada*

There are plenty of electronic structure theory approaches to tackle the quantum many body problem, each with their own pros and cons. Some aim to work for larger systems at the expense of accuracy while others aim the vice versa. All many body methods have been developed with the ground state in mind therefore excited state processes are difficult to model. Our new approach known as Fermionic Molecular Dynamics method hopes to fill this void as it lies in the middle of the spectrum of molecular dynamics method being semi classical in nature it can better deal with higher state excitation processes. In this study we applied FMD on few systems such as the hydrogen atom, dihydrogen cation and modelled the scattering theory via FMD results were well within the literature and it provided some invaluable insights about the time dynamics of the electrons. Overall, the tests were very promising showing that the method can be applied on multi electron systems with some possible improvements.

P18 | Developing Transferable Neural Network Potentials with Improved Accuracy, Applicability, and Interpretability

Leila Pujal *Queen's University, ON, Canada*

Characterizing the energetic landscape of large molecules is crucial for understanding and predicting the behavior of (bio)chemical systems. Machine learning approaches circumvent the prohibitive cost of computing accurate molecular energies directly. Specifically, deep neural networks (DNN) with chemically invariant architectures have achieved impressive accuracy on diverse datasets of small-to-medium sized molecules. However, one of the main shortcomings of existing models is their poor transferability to larger chemical systems where long-range interactions are critically important. This presentation tackles the shortcoming of existing DNN potentials by shifting from the field's relentless focus on improving algorithms to improving the quality and quantity of the data. Specifically, we augment the training data with local information that is transferable by nature and test our model's ability to go beyond the training chemical space to predict the energies of larger molecules.

P19 | Design of bioactive molecules with machine learning methods using topological descriptors of the electron density

David Ramirez-Palma *Centro de Investigación y de Estudios Avanzados del Instituto Politécnico Nacional, YUC, Mexico*

The combination of machine learning models (i.e. predictive models) and molecular models (i.e. docking, molecular dynamics simulations) has been used for the design of bioactive molecules. Advances in molecular representation of small molecules and the binding recognition process, towards a single or multiple targets, has sparked the interest of the scientific community in novel strategies of artificial intelligence aiming to solve three fundamental problems: 1) the number of possible interactions between a set of ligands and a specific protein, 2) the number of possible receptors that a single ligand may have, and 3) the myriad of ligands and proteins in a complex biological system. The importance of developing accurate methods for the description of ligand-receptor interacting patterns becomes apparent. In this work we develop predictive models of ligand-receptor interactions based on machine learning methods and using descriptors derived from topological analysis of the electron density, QTAIM. We expect that this approach will help reducing the occurrence of false positive and false negative in the search of bioactive molecules in a fast and efficient manner.

P20 | Path Integral Monte Carlo Approach for rotors using a Discrete Variable Representation and Gibbs Sampling

Wenxue Zhang *University of Waterloo, ON, Canada*

The Path Integral Monte Carlo (PIMC) method is efficient approach for the simulation of many-body systems. We present a novel PIMC-based algorithm with discretized continuous degrees of freedom and rejection-free Gibbs sampling. The method is applied to molecular rotations. The ground state properties of a chain of planar rotors with dipole-dipole interactions are used to illustrate the approach. Energetic and structural properties are computed and compared to exact diagonalization and Numerical Matrix Multiplication for systems consisting of 2 and 3 rotors. The systematic Trotter factorization error is studied. For larger chains with up to 100 rotors, Density Matrix Renormalization Group (DMRG) calculations are used as a benchmark. We show that using Gibbs sampling is advantageous compared to traditional Monte Carlo-Hastings rejection importance sampling. Indeed, Gibbs sampling leads to lower variance and correlations for the computed observables. Consequently, less Monte Carlo steps are required for a given simulation with our new approach.

P21 | Symmetry adapted linear combinations of Gaussians for efficient photochemical dynamics simulation

Alex MacDonald *Dalhousie University, NS, Canada*

The nonadiabatic dynamics of internal conversion photochemistry involves strong coupling between molecular electronic states mediated by vibrational modes of atomic nuclei. The simulation of photochemical dynamics requires a quantum mechanical treatment of the atomic nuclei in addition to the electrons due to the ultrafast (fs-ps) timescales involved, which comes at a high computational cost. ”On-the-fly” dynamics methods use Gaussian trajectory basis functions to keep the basis size small for a moving nuclear wavepacket, however such methods typically do not take advantage of point group symmetries of molecules. We show how generation of symmetry adapted linear combinations of the Gaussian basis gives a more accurate, symmetry-preserving wavefunction with nearly the same computational cost as the non-symmetrized basis. Our methods demonstrate how symmetrization captures important quantum effects such as geometric phase effects that may be poorly described by an asymmetric basis.

P22 | If it Doesn’t Exist, Build it: An Invertible, Invariant Crystal Encoding for Generative Machine Learning and Application in Generative Machine Learning

Andrew White *University of Ottawa, ON, Canada*

Generative machine learning (ML) in chemistry requires a machine-interpretable encoding of chemical structures which is both invertible—meaning that the original structure can be reconstructed from the encoding—and invariant—meaning that each unique structure corresponds to a unique encoding, irrespective of rotation, translation, or other coordinate transformations. While this is a solved problem for molecular species, unique challenges associated with crystalline materials (periodic boundary conditions, loss of degrees of freedom, arbitrary lattice vector orientation/placement) have remained an obstacle to developing a suitable encoding for generative ML for crystalline materials. Extant crystal encodings must typically sacrifice invariance for invertibility, or compromise the level of invertibility to preserve chemical invariances. Many have soft or hard limits on the total number or type of atoms which can be accommodated, or require geometry optimization during decoding. With the goal of enabling generative ML for periodic solids, we present a novel crystal graph encoding based on chemically meaningful internal coordinates. The full crystal geometry is encoded, ensuring full invertibility without invoking a DFT or empirical structure relaxation. The use of internal coordinates preserves invariances to coordinate transformations. Uniquely among invertible crystal encodings, our internal-coordinate crystal graphs are additionally invariant to the choice/orientation of lattice vectors in the input structure. We demonstrate and validate the invertibility of our encoding on both small inorganic crystals and more challenging metal-organic frameworks (MOFs). The utility of the internal-coordinate crystal graph encoding is explored in a generative ML application, using a variational auto-encoder approach to generating hypothetical MOF structures.

P23 | Structure and dynamics in 1-ethyl-3-methylimidazolium bis(trifluoromethanesulfonyl) imide ionic liquid/carbonate co-solvent mixtures potential candidates for next generation Li-ion battery electrolytes– combined DFT and molecular dynamics study

Abraham Molla Wagaye *Addis Ababa Science and Technology University, Ethiopia*

The limited safety of current organic-based electrolytes for lithium ion battery (LIB) technology represents a major drawback of commercially available LIBs. For these reasons, there has been considerable research interest to replace the organic-based solvents in LIB with ionic liquids (ILs). Both DFT and MD simulations were used to study the structure and dynamics of 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide ionic liquid in the presence of ethylene carbonate and dimethyl carbonate co-solvent mixtures. In order to give a visual understanding of the molecular interactions, the structures of cations, anions, and cation - anion ion pairs were systematically studied using DFT calculations. The nature of hydrogen bond interactions in a series of ion pair conformers have been thoroughly discussed by analysing the interaction energies, stabilization energies and natural orbital analysis of the ion pair conformers. According to the MD study, the addition of carbonate co-solvents into the pure ionic liquid creates a more structured system than the pure ionic liquid. Furthermore, the behaviour of the MSDs for the centre-of-mass of the ions as a function of IL/carbonate co-solvent mixtures indicated that the ions exhibited slow dynamics (diffusivity) with higher carbonate content. Our study on the diffusion coefficient analysis of Li$^+$, [FSI]- and [TFSI]- ions have revealed that the organic solvents restrict the free motion of the ions, reducing the dynamics (diffusivity) of the electrolytes. The simulation results also revealed that the total molar ionic conductivity for the different mixing ratios of IL/carbonate blends decrease with higher contents of EC/DMC co-solvents.

P24 | Parametrization of a Molecular Excitonic Quantum Battery Model

Harold Mena *University of Alberta, AB, Canada*

Quantum batteries store energy in long-lived excited states. Owing to their quantum nature, it has been posited that they may exhibit faster charging/discharging than conventional electrochemical batteries. Although the majority of the research on quantum batteries has been theoretical, there have been a few preliminary experimental demonstrations of this ground-breaking concept [1]. Previously, using a generic Frenkel exciton model coupled to two thermal reservoirs, we demonstrated that symmetry-protected dark states may be used to store excitation energy indefinitely without loss to the reservoirs [2]. In this study, we construct a specific model using anthracene and pyrene molecules to occupy the six sites of the quantum battery models.

At the TDDFT level and employing a well-established electronic energy transfer (EET) model, we calculated the first-excited state energies of the six monomers and their corresponding inter-monomer couplings, accounting for the fact that each monomer is embedded in a hexamer. The results facilitate the identification of the desired symmetry-protected dark state and reveal possible strategies to for discharging the energy from the excited state. The first-excited state energies and electronic couplings will be used to parametrize a Frenkel exciton Hamiltonian, which will in turn be used to perform exciton dynamics simulations of the quantum battery.

[1] F. Campaioli, et. al. (2023). *Colloquium: Quantum Batteries.*
[2] J. Liu, D. Segal & G. Hanna, J. Phys. Chem. C123, 18303.

P25 | Simulating Optical Spectra using DFT/MRCI

Teagan Costain *University of Ottawa, ON, Canada*

We here report two new electronic structure methods that have been developed for the computation of ground and excited state energies which reproduce FCI and near-FCI results within 0.2 eV for valence excitation and reproduce reference CCSDT results within 0.4 eV for core excitation. These methods have been developed within the density functional theory and multi-reference configuration interaction (DFT/MRCI) framework, a semi-empirical level of theory that combines density functional theory (DFT) and wavefunction theory (WFT) for their respective strengths in describing dynamic and static correlation. The continued development of this electronic structure method is motivated by an increased interest in following the latest experimental studies in ultra-fast dynamics; the DFT/MRCI approach has been demonstrated in the literature to possess the advantages that it is i) black-box, ii) multi-reference, iii) computationally efficient, and iv) accurate. We presently describe a formulation of the DFT/MRCI Hamiltonian that is more general for accurate simulation of both UV-Vis and X-ray spectroscopy. This is made possible, in part, by taking advantage of the high-quality benchmark-level data made publicly available within the QUEST database. Fitting the empirical parameters of the modified Hamiltonians to reproduce purely ab initio electronic excitation energies herein yields a highly accurate and efficient method for the simulation of experimental spectroscopies.

P26 | Digital quantum simulation of molecular absorption spectra without the Born-Oppenheimer approximation

Sohan Sanjeev *Dalhousie University, NS, Canada*

The advent of quantum computing has come with the promise of quantum chemistry simulations with an improved scaling relative to classical computing methods. Whereas most proposals and demonstrations for quantum chemistry algorithms on quantum computers have focused on electronic structure, the low scaling cost for the simulation of physical systems means that nuclear degrees of freedom may be included on the same footing as the electrons, resulting in a pre-Born-Oppenheimer simulation. Without Born-Oppenheimer potential energy surfaces, the interpretation of results is based largely on physical observables of the wavefunction. We show how to extend previous methods for the time-domain quantum simulation of spectra to a pre-Born-Oppenheimer wavefunction ansatz. In particular, we compare approaches to represent the dipole operator in our simulation to enable the accurate simulation of spectra with all vibronic coupling effects included.

P27 | Limitations of Kohn-Sham DFT in 3:5 semiconductor materials: A comparative computational, XPS, and NMR approach

Aiden Farrant *Dalhousie University, NS, Canada*

Binary pnictogenides of aluminum crystallize in a high symmetry space group, making them suitable as a benchmark set for novel developments and applications of quantum chemical simulation and modelling methods. Interestingly, we have found that current methods for calculating chemical shifts, the primary observable in a nuclear magnetic resonance (NMR) experiment, fail for these systems with increasingly heavy anions. Agreement with literature examples and in-house experimental NMR data shows that discrepancies with theory increase as the anion is switched from P through As to Sb. Furthermore, we have found that multiple approaches within standard Kohn-Sham density- functional theory fail in the same way and are unable to reproduce experimental results. After testing with a variety of functionals to improve agreement with experimental band gaps, a known issue with DFT simulations, and inclusion of spin-orbit coupling, we were unable to improve agreement with experimental NMR data to a satisfactory degree. This failure indicates that discrepancies are likely arising from causes other than just the incorrect energy levels of the conduction bands. Instead, we posit that the inaccurate energy ordering of both valence and conduction bands, in particular low-lying semi-core states, may be the culprit. In this work, we attempt to use approaches beyond standard Kohn-Sham DFT, in particular the GW correction, to obtain improved electronic structures of these simple materials. Whereas the most prolific use of DFT involves solving the Kohn-Sham equations for each state by treating all the other possible electrons in the system as a static, non-interacting potential with the same density as the real system, the GW approximation goes further. The GW approach incorporates propagative interactions and treats some pairwise electron-electron interactions directly, allowing for improved modelling of properties dependent electron density at the nucleus and band energies of semi-core states. We show that in most cases, a GW correction improves agreement between calculated and experimentally reported band gaps. We also show, with accompanying valence X-ray photoelectron spectroscopy (XPS) experiments, that the true energy levels of semi-core d-states on Sb and As anions are more appropriately positioned relative to experiment. The connection of this approach to NMR shielding calculations is on-going.

P28 | Charge transfer excitations with constricted variational density functional theory as an alternative to TDDFT: A benchmark study

David Samuvel Michael *University of Manitoba, MB, Canada*

Charge transfer (CT) excitation processes are fundamental to the performance of organic light emitting diodes, photocatalysis, photosynthesis, etc. Computational protocols to capture CT in organic molecules and transition-metal complexes typically employ TDDFT within the adiabatic approximation due to its relatively low computational cost as opposed to wavefunction methods. TDDFT treats excitations as a perturbative calculation of the ground state time- or frequency-dependent polarization. However, standard local and GGA functionals do not capture the physics of a charge transfer excitation precisely, resulting in underestimation of the excitation energies. Some improvement is seen when a portion of exact exchange is included, which can be further corrected by range-separated hybrid functionals. Earlier, Ziegler et al. [1] proposed constricted variational DFT (CV-DFT) for the description of electronic transitions wherein the excited states were variationally treated, as opposed to perturbative treatment of time and frequency within adiabatic TDDFT. This method yielded comparable excitation energies for GGAs and hybrid functionals with reference data after a variational (SCF) treatment of the excited states [2]. In this contribution, we have applied the CV-DFT approach to benchmark CT excitations [3] against high-level ab initio reference data. Based on preliminary findings, the SCF-CV(8)-DFT methods affords excitation energies for BP86, B3LYP, PBE0 with RMSD of 0.58eV, 0.28eV and 0.30eV, respectively to CCSDT data. Furthermore, the method is comparable to the performance of TDDFT using double hybrids and range-separated hybrids.

[1] T. Ziegler, et. al. (2009) J. Chem. Phys. 130, 154102
[2] A. Ambrosetti, et. al. (2014) J. Chem. Phys. 140, 18A502
[3] D. Mester & M. Kállay (2022) J. Chem. Theor. Comp. 18, 1646

P29 | The study of molecular properties and electronic structure of of Amino Acid Ionic Liquids

Abolfazl Ashrafi *Shiraz University, Iran*

In this research, a novel group of amino acid ionic liquids were studied by using density functional theory. The interaction between these amino acid-based anions and four imidazolium-based cation were theoretically explored. In this respect, the conformers of each cation and anion were simulated. The molecular properties and electronic structure of each conformers have been investigated using conformational and energetic analysis, atoms in molecules topological parameters and natural bond orbital analysis. The results demonstrate that in addition to H-bond interaction other types of interactions between cations and anions have been also contributed. The interaction between DMIM cation and Gly anion is more stable than the interactions between other cations and anions. The values of calculated properties elucidate that oxygen atom of Gly forms stronger H-bond with H'C_6 of ring than with H' methyl or methylene groups of cations. Different correlations have been obtained between calculated properties and glass transition temperature (T_g). Among various properties, electronic density shows the best correlation with T_g with correlation coefficient 0.881 whereas the worse correlation is found for the energy of hydrogen bonding.

P30 | Predicting the aqueous pKa of opioids and fluorinated derivatives

Clara Cunha *Thompson Rivers University, BC, Canada*

The misuse of opioids to relieve acute pain has led to an overdose crisis in North America without precedent Most opioids are protonated when they reach the blood stream (if their pKa is greater than the physiological pH of 7.4) and can couple to any opioid receptor. Inflamed tissue has a lower pH ($6.0 - 6.5$) due to acidosis. Hence, it has been suggested that reducing the pKa of the protonated tertiary amine group of an opioid by selectively replacing a hydrogen with a fluorine atom in certain positions, could increase its affinity to the opioid receptors associated with the inflamed tissue and reduce addiction, while not significantly altering molecular shape. Some experimental and theoretical work has been done in this regard, and it has resulted in the synthesis of novel fentanyl derivatives with promising pharmacological properties. Working with 37 protonated opioids, which includes some fluorinated derivatives, with experimental aqueous pKa values, theoretical methodologies for predicting this property have been developed. Five DFT functionals combined with continuum solvation models were tested. The best correlations between the calculated aqueous Gibbs energy difference of the acid and its conjugate base with the experimental pKa values produced a mean absolute error (MAE) of 0.43 pKa units ($R2 = 0.62$). Furthermore, 23 molecular descriptors corresponding to the 37 opioids were investigated making use of several machine learning methods: multivariable linear regressions, principal component analysis and principal component regression. The best preliminary results are obtained from a multivariable linear regression model involving three descriptors ($\mathrm{MAE} = 0.31$, $R2 = 0.83$). Adding more descriptors improves the predictive power of the equation, but high inter variable correlation becomes an issue. Using both approaches, aqueous pKa values are predicted for 32 new opioids and fluorinated derivatives, of which 10 appear to have pKa values in the desired range of 6.0 – 6.5 and might be good candidates for further studies. The knowledge acquired shows potential in enhancing opioid formulations.

P31 | Enhancing Exciton Transfer Efficiency in a Quantum Battery via Architecture Engineering

Zohreh Khodadad *University of Alberta, AB, Canada*

One of the key challenges in designing a quantum battery—a device that utilizes quantum states for energy storage and release—is to enable the quantum system to interact with its environment while maintaining its functionality. Our group proposed a strategy that leverages the dark states of a disorder-free quantum network with site exchange symmetries. It was demonstrated that an exciton could be indefinitely stored in such a dark state while preserving the symmetries and extracted from the network by attaching a thermal bath to break the symmetries. In this study, we investigate the effects of excited-state dissipation and dephasing on the exciton dynamics in the same six-site quantum battery model, using the Lindblad master equation. Our results show that during the storage phase, the dissipation and dephasing do not cause exciton leakage out of the dark state. However, during the discharge phase, the dissipation induced by the thermal baths impairs exciton transfer to the sink attached to the exit site. To address this challenge, we propose a new architecture where the sink is connected to site 3, to simultaneously break the symmetry and harness the exciton, instead of attaching a thermal bath to sites 2 and 3. This modification leads to a higher exciton transfer rate to the sink compared to the original design. Our finding suggests a strategy for enhancing exciton transfer rates during the discharge phase, particularly in more general cases where dissipation is present.

P32 | MEPO-ML: A Robust Graph Attention Network Model for Rapid Generation of Partial Atomic Charges in Metal-Organic Frameworks

Jun Luo *University of Ottawa, ON, Canada*

Metal organic frameworks (MOFs) are a class of nanoporous materials composed of inorganic nodes and organic linkers, which have attracted significant attention as the next-generation solid sorbents for gas separation applications such as CO_2 capture. Gas adsorption performances of MOFs can be evaluated by atomistic grand canonical Monte Carlo (GCMC) simulations; in high-throughput studies, accurate GCMC results are usually bottlenecked by the acquisition of partial atomic charge parameters, which requires a DFT calculation on a per MOF basis. As such, MOF screenings often use empirical charge sharing (e.g., QEq) models that generate charges in seconds but sacrifices accuracy. Recently, machine learning (ML) models have been trained to rapidly generate charges that achieve DFT-quality, where they were trained on $> 3,000$ MOFs obtained from the CoRE MOF database. However, recent reports have shown high structural error rates in CoRE. In this work, utilizing the extensively structure checked ARC-MOF database containing 279,632 MOFs with over 40 million DFT-derived ESP charges, a graph attention network for predicting partial atomic charges in MOFs was developed, referred as the MEPO-ML model. MEPO-ML was compared to other ML models reported in the literature. Using the same training set and descriptors MEPO-ML gave the lowest MAE of $0.025e$ on our test set of over 27K MOFs. Furthermore, gas adsorption properties of CO_2 and H_2S evaluated using MEPO-ML charges are found to be in significantly better agreement with results using the reference DFT-derived ESP charges compared to the empirical charges.

P33 | Analysing the Conformational Properties of Furanosides with Path Integral Molecular Dynamics

Megan Dawson *University of Waterloo, ON, Canada*

Monosaccharides, also known as simple sugars, are the smallest carbohydrate units that can be linked together to form carbohydrates. Cyclic monosaccharides with five-membered rings, known as furanoses, possess a greater degree of flexibility compared to their six-membered analogues. One challenge of sampling the conformations of furanoses is the long simulation time required to capture the conversion between conformations. Since these conformations are experimentally deduced from the vicinal proton-proton coupling constants (3JH,H) obtained with nuclear magnetic resonance spectroscopy (NMR), an additional challenge is the inclusion of nuclear quantum effects arising from the low mass of hydrogen. To address these challenges, we present a formalism for Path Integral Molecular Dynamics (PIMD) with umbrella sampling. PIMD captures nuclear quantum effects, while umbrella sampling is a non-Boltzmann sampling method that reduces the required simulation length by accelerating the rate of conformational change. A preliminary conformational analysis of L-arabinofuranose from PIMD and classical molecular dynamics simulations is presented, illustrating the impact of nuclear quantum effects on calculated coupling constants, 3JH,H, as well as the endo- and exocyclic rotamer populations for L-arabinofuranose. Each of the calculated vicinal proton coupling constants are compared to those from NMR. Future work will use the combined path integral and umbrella sampling approach, where the configurational space of L-arabinofuranose will be explored over shorter timescales. This will open the door to simulations of larger oligosaccharides systems.

P34 | Insights into the Structural Dynamics of Modified Thrombin Binding Aptamers: A Molecular Dynamics Study

Makay Taylor Murray *University of Letbridge, AB, Canada*

Aptamers are single-stranded nucleic acids, typically 15–100 nucleotides long, that can be designed to bind with high affinity and specificity to a wide range of targets (e.g., small molecules, proteins, metals, or entire cells). Aptamers rival antibodies due to their small size, high chemical stability, and the potential for precise modification with reduced manufacturing cost. Although canonical nucleic acids have a limited library of building blocks (nucleotides), their chemical landscape can be expanded, and aptamer function enhanced, with modifications. Despite an abundance of studies on the impacts of modifications on nucleic acid structure and function, structural explanations for observed changes in the macroscopic properties upon nucleotide modification are lacking, which limits our ability to rationally design modified aptamers. The present work employs molecular dynamics (MD) simulations and the prototypical aptamer used to investigate the effects of modifications on aptamer function, namely the thrombin binding aptamer (TBA), to understand the structural dynamics of modified aptamers and rationalize experimentally-reported stabilities and target binding affinities. This poster will explore our recent work on several families of modifications, including those mimicking amino acids and saccharides as well as those designed as internal fluorescent probes, which were added in a variety of positions. The synergistic impact of more than one modification will also be investigated. By studying a diverse set of modifications at the atomic level, our work uncovers unique aptamer design principles that highlight different aptamer–target binding orientations, networks of strengthened interactions, target conformational changes, and novel nucleic acid structural motifs. Collectively, our studies will aid the future development of new aptamers with chemically-modified nucleotides for applications in medicine and biotechnology.

P35 | Vibronic Spectra of *cis*- and *trans*-Stilbene: A Quantum Dynamics Study

Tuong Huynh *University of Ottawa, ON, 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 $\pi\pi^*$ states, and the excited state dynamics of each molecules, are also examined in our study.

P36 | Computational Insight into the Impact of Tobacco Smoke-Induced DNA Phosphate Modifications on the Nucleosome

Rebecca Jeong *University of Lethbridge, AB, Canada*

DNA contains the genetic information within a cell. Unfortunately, modifications to DNA can occur at many different positions upon exposure to harmful agents in our environment. These modifications include formation of bulky DNA adducts. A common class of DNA damaging agent that results in a variety of adducts is nitrosamines, which are found in tobacco products among other sources. Out of the known carcinogens in tobacco, the most potent carcinogen is 4-(methylnitrosamino)-1-(3-pyridyl)-1-butanone (NNK), which has been found to cause lung cancer in all species tested regardless of the administration method. In cells, NNK results in the covalent attachment of alkyl groups to DNA nucleobases and the phosphate backbone to form pyridyloxobutyl (POB) adducts. Currently, there is limited information about how such modifications affect DNA structure and cellular function, particularly for backbone lesions and when eukaryotic DNA is packaged into chromatin that is made up of nucleosome core particles (NCP). When DNA is wrapped around a histone octamer in an NCP, the accessibility of damaged DNA for replication and repair becomes hindered. In this research, molecular dynamics (MD) simulations were performed on an NCP containing POB adducts formed at the DNA backbone with varying sequences (i.e., T as the 3' nucleobase and A or T as the 5' nucleobase). The structural insights gained from this work provide the first glimpses of the biological impact of bulky, flexible modifications to DNA in the NCP, which will inspire future studies to further understand their mutagenic consequences and connections with diseases such as cancer.

P37 | Comprehensive analysis of hydrogen bonds in Shape Memory Polymers by means of computational chemistry methods

Yuliia Didovets *Jagiellonian University, Poland*

Shape Memory Polymers (SMPs) are a large group of promising materials with the unique ability to "switch" between directly determined temporary shapes as well as recover their permanent shape. The reason for the great scientific interest in SMPs is the possibility to control the shape memory property by external conditions, such as temperature, light irradiation, and chemical environment. Specific PolyUrethane Copolymers (PUCs) satisfy the necessary conditions for a material to show shape memory properties. Firstly, PUCs have a two-segmented structure ensuring both the fixing (Hard) and switching (Soft) Segments. Secondly, PUCs are known for forming interchain hydrogen bonds, the reversible interactions. The breaking-formation of hydrogen bonds makes PUCs perfect systems for shape memory properties. Various experiments proved the important role of hydrogen bonds between the Hard Segments of polyurethane copolymers. This research work aims to deeply analyze the relationship between the chemical structure of the Hard Segment and the nature of formed hydrogen bonds. Quantum chemical calculations were performed in ADF and CP2K software. The reorganisation of interchain hydrogen bonds was analysed by molecular dynamics of model systems, while the character and strength of formed hydrogen bonds were investigated by the Ziegler-Rauk energy decomposition scheme. The evaluation of results was additionally supported by comparison with the experimental spectroscopic and thermal measurements. The overall conclusions show clear dependences between the chemical structure of the Hard Segment and the interchain interactions' character.

P38 | Molecular Modeling of the μ-Opioid Receptor Complexed with Carfentanil Analogs

Savannah Mercer *Vancouver Island University, BC, Canada*

The number of drug-related fatalities due to synthetic opioids like carfentanil are increasing in BC and across Canada [1]. One strategy to reduce the number of opioid-related deaths is the implementation of harm-reduction checking sites, where people can bring samples to be tested for the presence of opioids and other toxic substances. Recent mass spectrometry analysis at these sites has found that samples that contain carfentanil are often contaminated with two previously unidentified compounds [2]. These compounds are thought to be synthetic precursors of carfentanil, and it is unknown if these precursors have similar toxic properties to carfentanil. In the body, opioid drugs bind to a receptor, known as the μ-opioid receptor (μOR), which induces both the desired physiological effects and the toxic side effects of opioids [3,4]. Therefore, studying how these precursors interact with the μOR will yield insight into their potential toxicity. In this work, a preliminary molecular docking study revealed that the two precursor molecules have similar binding poses as carfentanil in the μOR, and they share similar binding energies.[2] However, molecular docking is a static computational technique which is done in the absence of solvent, and a dynamic approach would provide us with a better insight into the biological activity of these precursors. Therefore, we performed long-timescale molecular dynamics simulations in order to determine more accurate binding energies of the two precursors and carfentanil to the μOR. Umbrella sampling was then performed to calculate more accurate binding energies of the molecules, and here we present our findings.

[1] BC Coroners Service. Illicit Drug Toxicity of Drug Data (to Dec. 31, 2022). Ministry of Public Safety and Solicitor General 2023.
[2] S. A. Borden et. al. (2023) Drug Test Anal. 15, 484.
[3] H. W. D. Matthes et. al. (1996) Nature 383, 819.
[4] G. W. Pasternak, et. al. (2013) Pharmacol. Rev. 65, 1257.

P39 | Kinetic Approaches to Nucleation

Richard Bowles *University of Saskatchewan, SK, Canada*

Nucleation is the process by which liquids crystallize during a first order transition. However, despite being an inherently kinetic process, most theoretical approaches focus on the thermodynamics of cluster formation, often using the bulk properties of the perfect crystal as ingredients. Our recent work explores approaches to nucleation that focus on the influence of the monomer addition and loss, and particle ordering kinetics on both the transient and steady state properties of crystal nucleation. In particular, we show that in cases of non-classical crystal nucleation, the interplay between the free energy surface and the microscopic ordering kinetics leads to distinct nucleation pathways where large, disordered clusters, appearing at intermediate times, may play either a direct or indirect role in crystal nucleation.

P40 | Comparison of DFT dispersion corrections on the DES15K database

Cameron Nickerson *Dalhousie University, NS, Canada*

While density-functional theory (DFT) remains one of the most widely used tools in computational chemistry, most functionals fail to properly account for the effects of London dispersion. Hence, there are many popular post-self-consistent methods to add a dispersion correction to the DFT energy. Until now, the most popular methods have never been compared on equal footing due to not being implemented in the same electronic structure packages. In this work, we performed a large-scale benchmarking study, directly comparing the accuracy of the XDM, D3BJ, D4, TS, MBD, and MBD-NL dispersion models when applied to the recent DES15K database of nearly 15,000 molecular complexes at both expanded and compressed geometries. Our study showed similarly good performance for all dispersion methods (except TS) when applied to neutral complexes. However, they all performed worse for ionic complexes, particularly those involving dications of alkaline earth metals, due to systematic overbinding by the base PBE0 density functional. Investigation of the largest outliers also revealed that only the MBD and MBD-NL methods demonstrate surprising errors for complexes involving alkali metal cations at compressed geometries, where they tended to significantly overbind. As we would expect minimal dispersion binding for such complexes, we further investigated the origins of these errors for the potential energy curve of a model cation-p complex. Overall, there is little to choose between the XDM, D3BJ, D4, MBD, and MBD-NL dispersion methods for most systems. However, the MBD-based methods are not recommended for complexes involving organic species and alkali or alkaline earth metal cations, for example when modeling Li^+ intercalation into graphite.

P41 | Bulk nanobubbles in aqueous and non-aqueous liquids: molecular simulations and theoretical models for their stability and mobility

Peter Kusalik *University of Calgary, AB, Canada*

Nanobubbles are gas-filled bubbles in water with diameters typically in the $\sim$ 100nm range. These nanoscale gaseous domains have only recently come under focused scientific investigation, and have been confirmed to exist in bulk aqueous solution and with more limited reports for some non-aqueous liquids. While several features of nanobubbles are consistently reported, most notably their unexpected stability over long periods, there remains considerable uncertainty and debate regarding the nature and properties of bulk nanobubbles. Nevertheless, bulk nanobubbles have aroused considerable interest across a wide range of real-world applications, from medical imaging to water treatment and agriculture. This presentation will begin by providing a more general overview of nanobubbles, their properties, and some of controversy surrounding nanobubbles and their unexpected features. It will then have a more detailed look into possible explanations for nanobubbles and their behaviour. Specifically, I will introduce a simple physical model that is able to account for both the stability and mobility of bulk aqueous nanobubbles. This model uses the polarization of the air/water interface, considering dipole and quadrupole contributions, together with the spherical bubble geometry to account for forces giving rise to both nanobubble stability and mobility. This presentation will also report some results from molecular simulations of bulk aqueous and non-aqueous nanobubbles. I will show that both short-range and long-range interactions in these systems must be treated with care. The predictions of the proposed physical model will be demonstrated to be fully consistent with results from these molecular simulations.

P42 | Nudged Elastic Band applications for reaction pathways

Julien Appleby-Milette *University of Victoria, BC, Canada*

Nudged Elastic Band (NEB) calculations are now the standard transition state calculation tool. The energies along the reaction pathway which are generated by NEB can also be combined along a more complex reaction pathway. Direct comparison of the reaction pathway energies for competing reactions gives a detailed account of the features which determine the selectivity and rate of reactions under different conditions. To ensure that binding energies do not introduce bias to the connection between sequential NEB calculations, we must ensure that the final product has full physical separation. In the following example, the NEB curves shown for the oxidation pathways of two Sn compounds show that the Beta-Hydride Elimination pathway is inhibited by a tetrahedral inversion. The Beta-Hydride transition is lower in energy than the competing hydrogen transfer mechanism but the inversion requirement on the Beta-Hydride Elimination makes the hydrogen transfer more favourable.

P43 | Using QM/MM and adaptively biased MD to study the debated MBD4 mechanism of action

Dylan Nikkel *University of Lethbridge, AB, Canada*

DNA is an important biological molecule that stores the majority of the genetic information of a cell. DNA is composed of four unique nucleobases, namely adenine (A), guanine (G), cytosine (C), and thymine (T). As a key part of epigenetic regulation, C is often methylated at C5 to form 5-methylcytosine (5-mC); however, this modified base can be deaminated, which results in a mutagenic T:G mispair. To prevent mutations, cells utilize the methyl-CpG binding domain 4 (MBD4) enzyme to detect and remove T in T:G mispairs. There is an urgent need for a better understanding of the MBD4 mechanism because of a correlation between MBD4 misfunction and cancer formation. However, the mechanistic pathway used by MBD4 is unclear, with conflicting crystal structures supporting different pathways. In this poster, the MBD4 mechanism is investigated using a combination of molecular dynamics (MD) simulations and QM/MM calculations. The full MBD4–substrate complex was modeled using the Amber force field, with adaptively biased MD calculations employed to investigate the dynamics of the active site and generate a Gibbs energy surface related to different conformations of active site catalytic residues. From minima identified on the Gibbs energy surface, QM/MM models were developed to map the catalytic mechanism. Overall, this work provides the first computational support for the MBD4 direct deglycosylation mechanism, with our predicted mechanism in excellent agreement with a wealth of experimental data. Thus, our work has resolved the mechanistic debate in the literature and provided structural information to aid the development of cancer treatments.

P44 | Photophysical behaviour of 2,2’-bipyridine-3,3’-diol: Fluorescence study in solvent mixtures using the ASEP/MD methodology

Nelaine Mora-Diez *Thompson Rivers University, BC, Canada*

The photophysical behaviour of organic molecules is pivotal for advancing in fields like photoelectronics. This research focuses on the excited-state intramolecular proton-transfer (ESIPT) of 2,2’-bipyridine-3,3’-diol ($BP(OH)_2$) in DMSO-water binary mixture. Ground- and excited-state geometries were optimized and characterized using density functional theory (DFT) and time-dependent DFT (TD-DFT), respectively, combined with continuum solvation methods for the pure solvents. Of the four levels of theory tested, B3LYP(PCM)/aug-cc-pVDZ produced the best results. Additional calculations in the pure solvents and in several binary mixtures were performed following the ASEP/MD methodology, which combines molecular dynamic simulations of the solute placed in a solvent box, with quantum mechanical calculations of the solute with solvent point charges from the MD simulation. It was found that the intramolecular proton-transfer in BP(OH)$_2$ occurs in the excited state after the most stable ground-state tautomer (the enol form) becomes electronically excited and emits green fluorescence radiation from the most stable tautomer in the first-excited state (the keto form). Both methodologies were successful in reproducing the experimental results: an intense absorption band at 340 nm and an emission band that shifts towards larger wavelengths with an increase in DMSO mole fraction. The insights gained from our research have direct implications for applications in fields such as organic electronics, photovoltaics, and fluorescence imaging. By understanding the fundamental process, we aim to contribute to the design of improved materials for various technological applications.

P45 | Observing Charge Transfer Dynamics in Molecules: First Principles Simulation of Valence and Core Spectroscopies of DMABN and its derivatives

Jibrael Rolston *University of Ottawa, ON, Canada*

Ultrafast photo-excitation generally leads to both electronic and geometrical (nuclear) rearrangements of a molecule's structure. One paradigmatic example is the twisted intramolecular charge transfer dynamics evinced by dimethylamino benzonitrile (DMABN). Here, the large amplitude motion, involving a twist and bend of the dimethylamino group, gives rise to a charge transfer state, characterized by a separation of charge between the benzene ring and the amino group. These nuclear and electronic rearrangements have served as a great benchmark for those testing the efficacy of their methods in detecting charge transfer states, and for those exploring the ability to achieve long lived charge separation in molecules. The wealth of studies on DMABN has also led to many conflicting interpretations of the nuclear structures and electronic configurations important to the excited state dynamics of the molecule. By probing the electronic structure of DMABN with simulated valence absorption and photoelectron spectroscopies, along with new core absorption and photoelectron studies, a series of specific novel time-resolved experiments were proposed to conclusively image the evolving charge transfer character in this system. Specifically, a dual X-ray Absorption and X-ray Photoelectron study on DMABN and its analogues is proven to be an efficient way to resolve signals attributed to charge transfer excited state minimums. This work demonstrates the effectiveness of a new quantum chemistry method in replicating experimental spectroscopies, DFT/MRCI(2). It was proven that said method is suitable for computationally inexpensive, core and valence absorption/photoelectron spectroscopies, while also retaining the ability to treat charge transfer states appropriately.

P46 | A Computational Investigation of Metal Binding to Modified Nucleic Acids

Briana Boychuk *University of Lethbridge, AB, Canada*

Metal ions play important roles in biology such as providing charge and structural stabilization to nucleic acids, and maintaining cellular functions and communication. Aside from participating in biological functions, metal–nucleic acid interactions have been exploited in therapeutics, nanomaterials, and biosensors. Indeed, nucleic acids have several properties that are advantageous in different applications, including metal binding specificity, thermodynamic stability, unique folding properties, and possessing multiple sites suitable for modification. The programmability of nucleic acids is particularly beneficial for enhancing metal–nucleic acid interactions in different applications, allowing for easy addition of chemical modifications to the sugar–phosphate backbone or nucleobases. Modifications that replace the canonical backbone are valuable for developing therapeutics, nanomaterials, and biosensors, primarily due to charge manipulation, which can alter metal binding trends and increase the resistance of nucleic acids to enzymatic degradation. One intriguing modified nucleic acid is peptide nucleic acid (PNA), which replaces the DNA/RNA sugar–phosphate backbone with a peptide backbone. In the present work, molecular dynamics (MD) simulations (AMBER) are used to gain insights into the preferred metal binding locations and the structural impacts of metal coordination to PNA in comparison to canonical DNA. An initial emphasis was placed on understanding Na^+, which is prevalent in biological systems, and Li^+, which requires solutions for environmental remediation and material recovery for battery technologies. The structural insights gained from this work provide fundamental information about metal–nucleic acid interactions in biology and ways to exploit modified nucleic acids in novel technologies.

P47 | Quantum Simulations of Water Chains under Nanoconfinement: from Carbon Nanotubes to Protein Channels

Jacob Chausse *University of Waterloo, ON, Canada*

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 with simulations, 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, preliminary work regarding quantum simulations of this system is presented, including the use of precomputed discretized potential energies and forces to accelerate path integral molecular dynamics simulations. The tools and methods developed to study the water-filled CNT will naturally lend themselves well to other confined water systems, and studying these could enable tuning of the currently observed quantum properties or uncover new ones. Aquaporins, a family of transmembrane water transport proteins, are one such confining structure, and they are of particular interest as the potential basis for organic quantum devices. Prospective research therefore includes efficient simulations of water chains in aquaporin proteins. This will allow for rapid study of the many aquaporins catalogued in the literature to assess whether aquaporins possess the quantum properties found in other water chain systems.

P48 | Computational Study on Photoswitching Mechanism of Cyanin-based Dyes

Mohammad Izadyar *Ferdowsi University of Mashhad, Iran*

The stability under light exposure holds significant importance for fluorophores. Those possessing remarkable stability find extensive utility across various domains, including bioimaging, theranostic, chemical sensors, and optoelectronics. In this research, we delve into a theoretical investigation of a photoswitch system based on Cyanine. Our computations have unveiled that photoisomer O (Open type) displays prolonged absorption and emission wavelengths in the UV-vis-NIR spectrum compared to its counterpart, photoisomer C (Closed type). Our computational analysis on the optoelectronic attributes of both O and C in their ground and first excited states indicates that isomer O exhibits lower energies for both excitation and de-excitation processes compared to its C counterpart, consistent with the observed elongation in absorption and emission wavelengths. To understand the differing quantum yields in water, we evaluated the transition tendency of these molecules to the non-emissive Twisted Intramolecular Charge Transfer (TICT) state. Fluorophores with polymethine bridges are prone to this state. C's lower quantum yield stems from its stronger TICT propensity, driven by favorable kinetics and thermodynamics. This state exhibits complete charge separation, contrasting with the Local Excited state's charge delocalization. C's rotation around the $C-C$ bond highlights its lower energy barrier (0.27 vs 0.39eV) and stronger driving force (1.30eV) compared to O (0.44eV), indicating enhanced TICT tendencies. This exploration clarifies the unique photophysical behaviors of the polymethine bridges of O and C, a crucial aspect in molecular engineering aimed at facilitating photoconversion into the dark state of cyanine-based photoswitches.

P49 | Introduction of Advanced Chemistry Program: Global Reaction Route Mapping (GRRM)

Kenshiro Kimura *HPC Systems Inc. Japan*

Global Reaction Route Mapping (GRRM) is an advanced computational chemistry software designed for comprehensive exploration of chemical reactions, potentially aiding in discovery of unexpected reaction paths. This software operates in conjunction with quantum chemistry calculation software which struggles to identify potential chemical reactions derived from single molecule information on their own, significantly enhancing their capability to do so through its original algorithms. The GRRM program has been continuously updated with various functions, evolving into its latest version, “GRRM23”, which enhances its utility in chemistry-related fields, including catalyst and battery research. These functions include Artificial Force Induced Reaction (AFIR) method for global reaction path searches, Rate Constant Matrix Contraction (RCMC) method for kinetic analysis, and Quantum Chemistry-aided Retrosynthetic Analysis (QCaRA) method for retrosynthetic analysis. This remarkable program was developed by Professor Maeda’s research group at ICReDD (Hokkaido University, Japan), and its license has been provided worldwide by our company, HPC SYSTEMS Inc.: a Japanese company that maintains a strong collaborative relationship with this group and is committed to providing high-performance computing (HPC) solutions with strength in computational chemistry to empower researchers. Additionally, recognizing potential need for a large amount of computational resources required for comprehensive reaction path searches in GRRM calculations, we are expanding implementation of this software on supercomputers internationally. This initiative aims to provide large-scale computing environment that enables researchers to explore vast amounts of chemical information in a short period.

P50 | Coordination Number Dependent Deposition of Cysteine on Nanostructured Au Substrates: A DFT study

Aishat Idris *University of Victoria, BC, Canada*

The adsorption of amino acids on nanostructured metallic surfaces has implications in many fields of science and engineering, particularly in health and sensing applications. A commonly studied interaction of this kind is cysteine on gold, as cysteine is the single proteinogenic aminoacid capable of chemically binding metallic substrates. Despite this interest, there are still uncertainties regarding the chemical behaviour of the S-Au bond in adsorbed cysteine, and the impact of surface unsaturation on this bond. In this work, we examine computationally the configurational space of cysteine adsorption on rough gold substrates, considering several distinct binding motifs. The structural, dynamic and energetic features of the thiol group binding, together with the surface interactions of other functional groups present in the molecule are considered for a series of adsorption sites of different in-surface coordination, using ab initio molecular dynamics and density functional theory calculations. Our results have applicability in understanding the structural features of cysteine motifs upon binding and the interactions of mercapto-aminoacid binding to defect substrates, as well as to ultimately inform coordination-dependent force fields that may be used in classical simulations of larger systems.

P51 | Molecular Dynamics Simulations of Adsorption of Phenol, Catechol and Gallol to Silica Surfaces at Different Concentrations.

Yifei Zhang *University of Alberta, AB, Canada*

Many aquatic organisms exhibit strong adhesion to rock surfaces. Understanding the molecular origins of this adhesion is crucial for controlling interfacial adhesion behaviour and developing adhesives that can be used in underwater environments. In this work, we performed molecular dynamics simulations to study the adsorption behaviour of three phenolic compounds (viz., phenol, catechol, and gallol) at the silica-water interface at different concentrations. The results show that the molecules are attracted to the silica surface, with the hydroxyl groups mainly oriented towards the surface. Based on the number of phenolic molecules near the silica layer and the number of hydrogen bonds, this attraction increases with the number of hydroxyl groups in the molecule (i.e., one for phenol, two for catechol, three for gallol). As the concentration of a phenolic compound increases, the attractive forces acting on individual phenolic molecules decrease, and the number of hydrogen bonds between the phenolic molecules and the silica layer saturates. The hydrogen bond autocorrelation function shows that as the number of hydroxyl groups in the molecule increases, the average strength of the individual hydrogen bonds between the phenolic hydroxyl groups and the silica surface remains constant, while the duration for which phenolic molecules remain on the silica surface increases. The insights gained from this study could be instrumental in designing new phenolic-based adhesives for silica-water interfaces.

P52 | An MP2 Study of Counterion Trapped Norcaradiene and Cycloheptatriene

Chen Liang *Ontario Tech University, ON, Canada*

Highly polar molecular systems, such as M-mol-X insertion complexes (M=alkali, mol=molecule, X=halide), offer a wide array of potential applications spanning light-matter interactions, optics, energy storage, transmembrane ion-pair transport, and molecular interactions. In this study, we employ computational methods to investigate the insertion complexes formed by norcaradiene and cycloheptatriene molecules confined between Na-I counterion pairs. Our analysis encompasses structural characterization, stability assessments, charge distributions, infrared spectroscopy predictions, and exploration of isomerization reactions. Notably, we examine the stability of these complexes and the influence of ions on the isomerization of norcaradiene into cycloheptatriene. Furthermore, we present calculated infrared spectra to aid in experimental detection. Overall, our findings contribute valuable insights into the behavior of insertion complexes, aiming to streamline the design and application of these systems.

P53 | Understanding the Enhanced Photocatalytic Activity of Se Doped Anatase TiO_2: A Theoretical Study

Niranji Thilini Ekanayake *Queen's University, ON, Canada*

Developing clean, renewable, and economically feasible energy sources is essential to meeting growing energy needs while ensuring environmental sustainability. Photocatalytic water splitting transforms water into hydrogen and oxygen using sunlight in the presence of a catalyst and is one of the most promising energy conversion systems for green hydrogen production. TiO_2 is one of the most popular and intensively studied water splitting photocatalysts. The use of pristine TiO_2 in this context is limited by this material's wide band gap of 3.2eV, which limits the absorption of visible light. Different strategies have been explored to improve the optical absorption of TiO_2 in the visible light region and impurity doping has been identified as one of the best strategies to improve the photocatalytic activity of TiO_2. Numerous studies have shown that doping with metals and non-metals can reduce the band gap by introducing mid-gap states. Although Se-doping on

TiO_2 has not been widely investigated, existing experimental studies indicate that Se significantly improves the TiO_2's ability to absorb visible light. In this work, we used DFT calculations to explore how replacing a range of O atoms in TiO_2 with Se affect the light absorption properties of this material with the goal of applying these insights to develop effective water splitting photocatalysts. The electronic properties, optical absorption spectra and spatial distributions of wavefunctions associated with low-energy excitations will be discussed.

P54 | A DFT investigation into several metal-dithiolene, -diselenolene, and -ditellurolene complexes to produce H_2 gas

Eric Bushnell *Brandon University, MB, Canada*

As a result of burning fossil fuels levels of greenhouse gases in our atmosphere are increasing at an alarming rate. Such an increase in greenhouse gases threatens our planet due to global climate change. To reduce the production of greenhouse gases we must switch from fossil fuels to alternative fuels for energy. The most viable alternative energy source involves the conversion of solar energy into chemical energy via the electrocatalytic splitting of water to form molecular hydrogen. In the present work the metal-dithiolene, -diselenolene, and -ditellurolene complexes were studied using Density Functional Theory (DFT) to investigate the thermodynamics and kinetics of the hydrogen evolution reaction. Key results will be presented.

P55 | DFT Studies of Glycerol on Bi-Modified β-NiOOH Surfaces

Shideh Ahmadi *Queen's University, ON, Canada*

Renewable fuels such as biodiesel offer promising alternative energy sources to combat climate change. However, biodiesel production results in a significant amount of glycerol as a by-product. Electrooxidation of glycerol to yield more valuable chemicals can reduce the costs associated with biodiesel. Here, we use computational explore the interaction between glycerol and β-NiOOH (001) surfaces as the first step in the glycerol electrooxidation reaction (GEOR). We explore the interaction involving pristine β-NiOOH (001) and that surface decorated with bismuth, a unique method that has been observed experimentally to activate the GEOR. The geometries of glycerol adsorbed on these surfaces, the adsorption energies, and charge density differences are also analyzed by testing various positions of bismuth on the surface to determine how glycerol adsorbs. This research aims to provide insights to enhance glycerol conversion and leverage biodiesel by-products to contribute to environmental sustainability and economic stability.

P56 |

Danish Khan *University of Toronto, ON, Canada*

The feature vector mapping used to represent chemical systems is a key factor governing the superior data efficiency of kernel based quantum machine learning (QML) models applicable throughout chemical compound space. Unfortunately, the most accurate representations require a high dimensional feature mapping, thereby imposing a considerable computational burden on model training and use. We introduce compact yet accurate, linear scaling QML representations based on atomic Gaussian many-body distribution functionals (MBDF) and their derivatives. Weighted density functions of MBDF values are used as global representations that are constant in size, i.e., invariant with respect to the number of atoms. We report predictive performance and training data efficiency that is competitive with state-of-the-art for two diverse datasets of organic molecules, QM9 and QMugs. Generalization capability has been investigated for atomization energies, highest occupied molecular orbital–lowest unoccupied molecular orbital eigenvalues and gap, internal energies at 0K, zero point vibrational energies, dipole moment norm, static isotropic polarizability, and heat capacity as encoded in QM9. MBDF based QM9 performance lowers the optimal Pareto front spanned between sampling and training cost to compute node minutes, effectively sampling chemical compound space with chemical accuracy at a sampling rate of molecules per core second.

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Jason Pearson	University of Prince Edward Island	`jpearson@upei.ca`	chair	12
Gilles Peslherbe	Concordia University	`gilles.peslherbe@concordia.ca`	chair	14
Piotr Piecuch	Michigan State University	`piecuch@chemistry.msu.edu`	invited	17
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Tom Woo	University of Ottawa	`twoo@uottawa.ca`	chair	16
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