Modelling 2D Amorphous Materials: The Curious Case of Monolayer Amorphous Carbon

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Amorphous materials are common, but they are poorly understood and potentially underutilized. As a class they are characterized by fast decaying spatial correlations and by rich sets of manifested motifs. The richness of accessible conformations makes simulating them on a computer a difficult task. We address this problem by formulating a new method based on a generative deep neural network that is trained on a set of small-scale samples available either through traditional simulations or through experimental imaging techniques. After training, this model generates new and unseen samples of arbitrary size at linear cost effectively solving the problem of large-scale simulation of such materials. We apply this method to simulate with atomistic resolution a recently discovered 2D material, the Monolayer Amorphous Carbon (MAC) - a topologically distinct variant of Graphene. In this talk, I will describe our new method, its application to MAC, and some of the chemical-physical properties of MAC nano-fragments: steady-state and laser-induced electronic conduction.