Nanotechnology and miniaturization are paving the way towards a more energy-efficient and sustainable future for humanity. Nanostructures are commonly employed for commercial electronics such as computer chips, solar cells and electromechanical devices. Nanoengineered materials, such as carbon nanotubes, are also finding their uses for structural and chemical applications, for instance drug delivery and in vivo molecular detection. Understanding interatomic interactions is a crucial step along the path to controlling and engineering nanoscale systems. Because of reduced dimensionality, these interactions are difficult to study directly using experimental techniques, and much of the knowledge that we possess about the nature of atomic-scale processes has been gathered from theory and simulation.

Simulating a nanoscale system at the quantum level is very computationally demanding, and so the computational physics community is hard at work on developing effective interatomic potentials (also known as “force fields”) which can reproduce quantum-mechanical potential energy surfaces. Unfortunately, “classical” potentials, based on closed analytical forms, fail at accurately reproducing many phenomena, such as bond breaking/formation, defect formation energies, etc. A promising route, and one that provides a compromise between accuracy and CPU cost, is machine-learning-based interatomic potentials. We have used such potentials to explain for the first time the growth mechanism and origin of the high degree of diamond likeness observed in tetrahedral amorphous carbon (Fig. 1). Ultimately, our objective is to run computational experiments which will expedite and reduce the cost of developing new nanomaterials and nanostructures, by allowing experimentalists to avoid the trial-and-error approach currently employed.

In this project, we will develop machine-learning-based potentials to study materials with important technological applications, for which reliable classical potentials do not exist. Initially, we will focus on elemental phosphorus and will use our new potential to study heat conductivity and other properties of 2-dimensional black phosphorus.

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