

STEM

Building Predictive Chemistry Models

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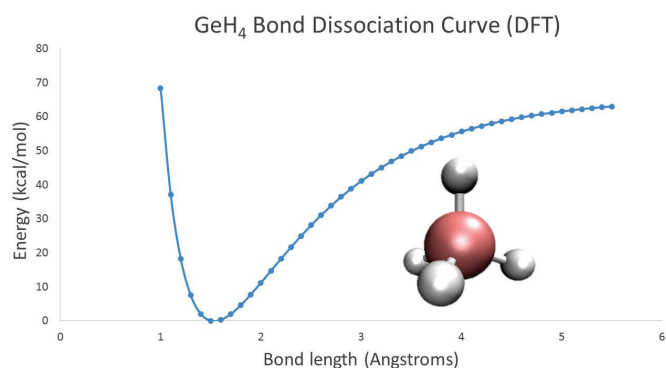
The completion of the theory of quantum mechanics in the 1920s created a framework from which physical and chemical laws could be fundamentally derived from theory. Such a theoretical tool has immense applications in accurately modeling complicated chemical systems, materials, and nanodevices. Density functional theory (DFT) is one computational method for solving the Schrödinger equation to model a chemical system of roughly one to one hundred atoms in size. The mathematical complexity of these equations, however, poses an extreme problem in actually using this deep theory. Even with the advent of powerful supercomputers, DFT remains slow and computationally expensive.

In an effort to widen the application of chemical modeling, molecular dynamics (MD) approximates the complicated chemical interactions between atoms with Newtonian-like forces. MD ignores the movement of electrons and instead characterizes bonding, van der Waals, Coulombic, and other intermolecular forces as a direct function of distance between atoms. These forces are approximated at several distances using DFT simulations, which provide very high-accuracy data to curve fit the molecular dynamics force field. By making this simplification, molecular dynamics can run much larger simulations several times faster. This allows for simulations of up to billions of atoms instead of hundreds, giving a much better representation of macroscopic processes.

This research set out to expand the functionality of ReaxFF, a particular equation model for molecular dynamics, by generating a data training set for copper oxides and germanium oxides. Metals are of particular interest in improving molecular dynamics simulation because of their complicated electronic structures, which make modeling with

Newtonian forces difficult. DFT simulations were used to generate the bond dissociation curves for several atom-atom pairs involving hydrogen and oxygen with either copper or germanium. Each dissociation curve was then compared to the molecular dynamics prediction, and Monte Carlo simulations were used to adjust the parameters of the MD force field until the model fit the DFT better. These parameters were published for other researchers to adapt into their simulations to improve the accuracy of copper-hydrogen-oxygen and germanium-hydrogen-oxygen interactions.

Graduate research advisor Nicolas Onofrio writes, "Molecular dynamics simulations allow for simulation of devices of interest in nanoelectronics; however, the limitation in parameters describing the interactions between atoms restricts the range of materials application. Christopher computed high-level theory data used to optimize molecular dynamics parameters for germanium, copper, and the respective oxides. As a result, this work will help understand the atomic mechanisms that govern the operation of emerging nonvolatile memory devices."



Bond dissociation curve for Ge-H bond in GeH₄. Data generated with DFT using Gaussian09 software, B3LYP functional, and ccVTZ basis set.

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