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Building Predictive Chemistry Models

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ABSTRACT

Density Functional Theory (DFT) simulations allow for sophisticated modeling of chemical interactions, but the extreme computational cost makes it inviable for large scale applications. Molecular dynamics models, specifically ReaxFF, can model much larger simulations with greater speed, but with lesser accuracy. The accuracy of ReaxFF can be improved by comparing predictions of both methods and tuning ReaxFF's parameters. Molecular capabilities of ReaxFF were gauged by simulating copper complexes in water over a 200 ps range, and comparing energy predictions against ReaxFF. To gauge solid state capabilities, volumetric strain was applied to simulated copper bulk and the strain response functions used to predict elastic constants, which were then compared against experimental data and ReaxFF predictions. Results suggest ReaxFF's predictions are fairly robust, making it useful for molecular simulations. Training ReaxFF with this data can improve the accuracy of molecular dynamics simulations, providing wider application of molecular modeling software.

KEYWORDS

Molecular Dynamics (MD), Density Functional Theory (DFT), ReaxFF, copper complexes, bulk modulus

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