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Molecular Exploration Tool

Weiyi Cao
School of Electrical and Computer Engineering, Purdue University
Nicolas Onofrio and Alejandro H. Strachan
Neil Armstrong Hall of Engineering, Purdue University

ABSTRACT

Density Functional Theory (DFT) which is based on quantum mechanics theory has been broadly used to compute the energy and the structure of molecules and solids. However, the DFT method is limited when running calculations for a large system and only thousands of atoms can be solved. Alternatively, Molecular Dynamics (MD) simulation can be used to investigate the properties of the atomic system for large systems in the classical mechanics approximation. When running the MD simulation, the electronic structure is approximated by Force Fields (FF) which can be parameterized against DFT calculations. Nevertheless, the accuracy of the MD results and the FF is suspicious for the scientists because of the variety and complexity of the FF. Hence, a free web-browser based tool has been developed to allow the user upload a force field, run MD simulations and compare the results with the DFT calculations. Users can select desired molecules and solids in the database, run MD simulation, plot the corresponding energies and visualize the atomic structures. So that users can find out if they can trust the FF results according to the comparison with DFT calculations.

KEYWORDS

Density Functional Theory, DFT, Molecular Dynamics, MD, Molecular Exploration, GUI, Material Science

REFERENCES

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