Molecular Exploration Tool

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Introduction

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.

Objective

Use Rappture to develop a user-friendly tool that can compare the FF results with DFT calculations. Users can search for the DFT calculations they want in the database and run MD simulations. They can visually compare the FF results with DFT calculations and determine if the results from Force Field are accurate enough. However, the tool cannot train the Force Filed with the DFT calculations now. The tool will be more useful if it has the ability to do the training for the Force Field.

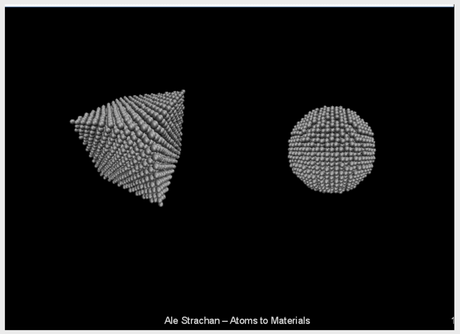

Figure 1. Molecular Dynamics

Molecular Exploration

The tool has 2 parts. The first part is a Molecular Exploration tool, and the second part is a Lammps Simulation tool.

For the molecular exploration tool, there is a database that contains many DFT calculations, and the user can search for the specific files that they want to explore in the database. The searching has the following constrains:

- Element Names: the user can type in the elements they are looking for with the first letter capital (example: “Si”). User can also choose to search for the files that only contain the selected elements or the files that have not only the selected elements but also other elements.
- Exchange Correlation Potential: the user can select the calculations that have been done with a specific functional (example. “PBE”)
- Structure Type: the user can narrow down the search to a specific type of structure (example: “Crystal”)

At the bottom of the interface, there is a selection that user can determine if they want to run the Lammps simulation on the selected structures. If the user choose ‘yes’, then the program will go to the second part of the tool and do the calculation.

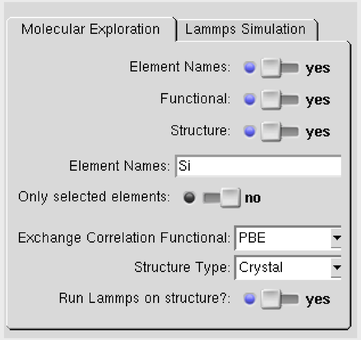

Figure 2. The interface for Molecular Exploration Tool

Lammps Simulation

For the second part, the Lammps Simulation tool, user can run the Lammps Simulation based on the selected XML files user has searched for in the database and compare force field with the selected DFT calculations. The tool has the following features:

- Users can upload their own force filed files or select one from the force field database
- If users only want to run the simulation on some of the XML files they just searched, they can type in the list of file names they want and separate each file by space. Otherwise, the program will run the simulation on all the files that match the users' constraints in the database.

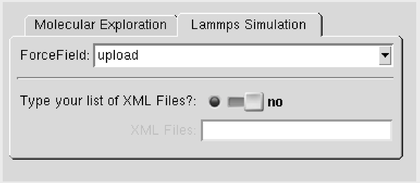

Figure 3. The interface for Force Field Calibration Tool

Molecular Exploration Results

The followings are the outputs for the Molecular Exploration Tool:

- Molecular Structure: a sequence of structures for different molecules. There will be a box around atoms for the crystal structure.

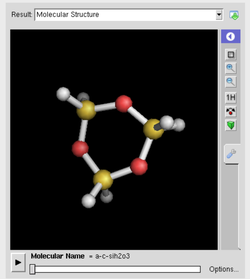

Figure 4. The structure for a-c-sih2o3

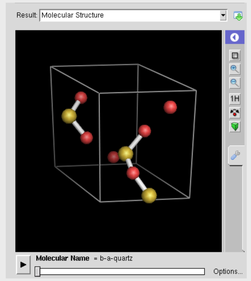

Figure 5. The structure for b-a-quartz (Crystal)

- Energy for different structures: a sequence of curves that are the plots of Bond Energy Vs. Steps for different molecules

Figure 6. The Energy plot for a-c-sih2o3

Figure 7. The Energy plot for b-a-quartz (Crystal)

- Sequences (animations) of molecule structures at different steps for the specified molecules: this output can show the responses of applying a force on the molecule, such as the dissociation of a bond and the torsion of an angle.

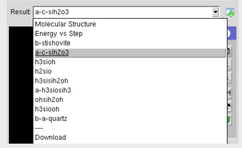

Figure 8. The lists of outputs

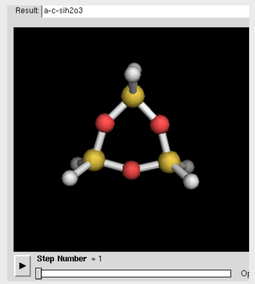

Figure 9. The molecule structure for a-c-sih2o3 at Step 1

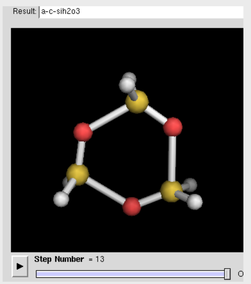

Figure 10. The molecule structure for a-c-sih2o3 at Step 13

Lammps Simulation Results

The followings are the outputs for the Lammps Simulation Tool:

- Energy vs Steps, plot the Energy vs Steps. Curves for Force Field and DFT on the same graph for each selected XML file. (The red line is for the Force Field, and the blue line is for DFT.)

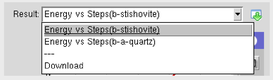

Figure 11. The list of plots for each selected XML file

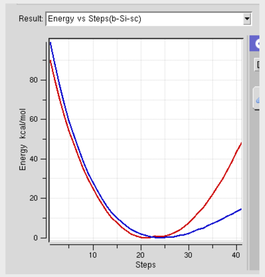

Figure 12. The Energy plots for Force Field and DFT (b-Si-Sc)

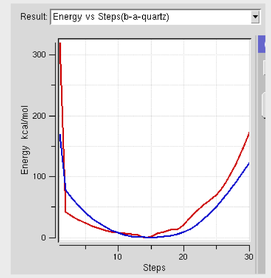

Figure 13. The Energy plots for Force Field and DFT (b-a-quartz)

Conclusion and Improvements

Overall, this tool has a user-friendly design and can be very helpful to Materials scientists and Chemical engineers who want to explore the atomic structures and figure out the accuracy of the Force Field. The Molecular Exploration can let users explore the atomic structures with different bond angles and bond distance. Also, the Lammps simulation results can help the user visually compare the FF results and the DFT calculations. Therefore, they can know the accuracy of the Force Field.

Although the tool is quite useful, it still has some problems that need to be solved. The first problem is that the simulation speed is not fast enough that users need to wait for a long time before the tool generates the results. One possible solution is to submit the calculations to the cluster and let the super computer run the simulation, which can be very quickly. The other problem is that users cannot get both results from Molecule Exploration tool and Lammps Simulation tool at the same time. This problem doesn’t have a possible solution if we use Rappture to build the tool. However, the problem is very likely to be solved if we use another tool to build the GUI, such as PyQt.

Reference

(2011), "Creating and Deploying Scientific Tools," https://hubzero.org/resources/381.
(2013), “From Atoms to Materials: Predictive Theory and Simulations,” https://nanohub.org/courses/FATM.