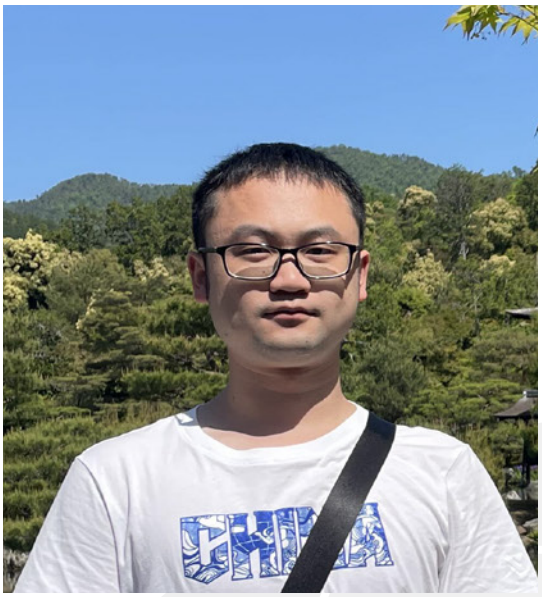
THE GEODYNAMICS SEMINAR № 622



Mr. Wenming Xia
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2024.10.25 (Fri.) 16:30 ~

Venue: Meeting Room #486
Science Research Bldg. 1, 4th floor.
Ehime Univ.

Machine learning model for the prediction of Hubbard U parameters and its application to Fe-O system & Fe-O-H system.

Without incurring additional computational cost, the Hubbard model can address prevalently the electron self-interaction problems of the local or semi-local exchange-correlation functions within density functional theory. However, determining the value of the Hubbard parameter, U, promptly, efficiently and accurately has been a long-standing challenge. Currently common methods like semi-empirical estimation by comparing with experimental or hybrid functional results, and the linear response constrained density functional theory (LR-cDFT) method all have limitations. Lack of experimental data and high computational costs make it difficult to apply these methods to complex systems such as disordered structures and to intricate processes such as structure search. However, Hubbard U parameter should not be treated as a fitting parameter as it is strongly influenced by local environment in strongly correlated systems. That is, Hubbard U parameter is affected by local crystal structures, such as bond lengths, bond angles, and polyhedral shapes, etc. We therefore advocate employing machine learning (ML) to establish a mapping between crystal structure and Hubbard U, resulting in the development of an efficient, fast, and accurate method for predicting the U parameter. This method performs well in calculating the properties of wüstite, hematite, and magnetite, aligning with experimental measurements or more costly hybrid functional results. At last, using this method, we redefine the convex hulls of the Fe-O system at 0, 50, and 100 GPa, the obtained results are in good agreement with experimental observations. We also find a new $Fe_2O_3H_2$ crystal structure at high pressure using this method combined with structure search.

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