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Development and Applications of Multi-Scale, Multi-Physics Simulators Based on Ultra-Accelerated Quantum Chemical Molecular Dynamics for Battery Technologies

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Introduction

Much attention has been given to battery systems, such as Li-ion battery, fuel cells, and solar cells. The design of such batteries has provided a variety of technological challenges to experimental researchers. For comutational or theoretical chemists also batteries have given a variety of theoretical challenges to contribute more from theoretical or computational view points. In collaboration with many experimental/industrial experts, the authors have tried to develop a variety of softwares for the design of batteries such as Li-battery, solar cells, and fuel cells. . In the present conference we describe method, accuracy, and performance of Ultra-Accelerated Quantum Chemical Molecular Dynamics(UA-QCMD) method for multi-scale, multi-physics simulations of battery technologies.

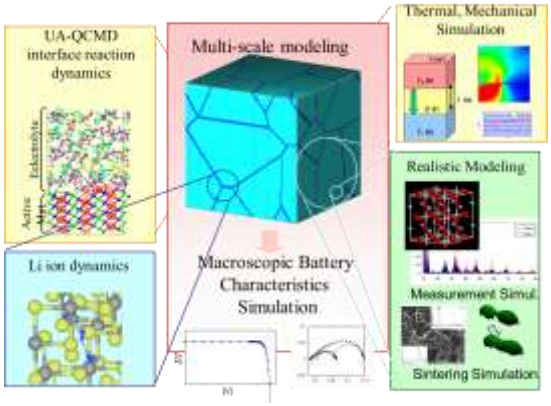

Fig. 1 Multi-scale, Multi-physics simulators of Li-ion battery.

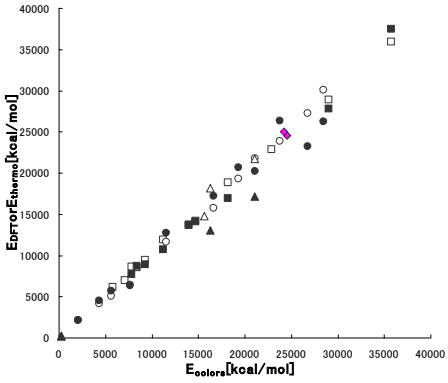

Fig. 2 Binding energy calculated by Colors(Ecolors) against that by DFT(E_{DFT}) and thermodynamic data (Ethermo) for various compounds.

Computational methods

Details of UA-QCMD method are described in our previous papers[e.g.1-4].

Results and discussion

In our previous studies UA-QCMD method with the first-principles parameterization is 10,000,000 times faster than the conventional first principles molecular dynamics method[3,4]. In the present study we demonstrated that the quantum chemical calculation in UA-QCMD, that is Colors, has high accuracy in comparison with DFT and thermodynamic data as shown in Fig. 2. In addition to the high accuracy in binding energy calculations, the UA-QCMD method can quantitatively reproduce the electron configurations of DFT calculations for various compounds. It should also be noted that the UA-QCMD is very effective for the electronic calculations of rare earth compounds with f-orbitals, while the DFT method cannot reach divergence easily and thus cannot converge for the compounds.

On the basis of high speed and high accuracy the UA-QCMD method has revealed dynamic structure changes under practical battery conditions. The validity of the dynamic calculations can be proved by simulating various spectroscopic results coupled with the comparison with experimental measurements. The precise determination of the geometry has determined nano-scale physical properties for mesoscopic and macroscopic Li-ion battery simulations(Fig. 1). The results of such multi-scale, multi-physics simulation were revealed to agree with various macroscopic measurements. Further details are described in the conference.

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