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Progresses of the hybrid quantum-classical simulation: development of O(N)-DFT method and application to Li-diffusion in graphite

Nobuko Ohba and Shuji Ogata

Summary

We have been developing the concurrent-type, hybrid quantum-classical simulation scheme for various atomic processes at liquid-solid interfaces [1]. In this scheme, the density-functional theory (DFT) method is applied to the "quantum" region to calculate the electronic structure; while the semi-empirical inter-atomic potential, to the "classical" region. In this talk we review its recent developments both from methodology and application viewpoints.

In the hybrid simulation, the DFT method that is applied at each time-step to a cluster of typically a hundred atoms (i.e., the QM region) consumes most of the computation power. It is highly desirable to develop a less compute-intensive scheme without degrading the accuracy of the original O(N3)-DFT. Motivated by this, we develop a novel O(N)-type, real-space DFT method for parallel machines. In this method a total QM region is describe as the superposition of the DFT sub-regions by introducing the density-template potential to each Kohn-Sham equation in addition to the embed-potential used in existing papers. The accuracy and performance checks are presented.

Theoretical understanding of the Li-diffusion is crucial for further advancement of the Li-ion battery. It is known experimentally that the Li distribution in the Li-graphite intercalation compound shows transitive stages as its density increases, called the stage structure; in each stage the Li-rich and poor layers align in a unique sequence. The Li-diffusivity varies by orders of magnitude depending on the stage. The open problems include the possible relation of the formation kinetics of the stage structure and the Li-diffusivity. Since the graphite expands locally by 10% when the Li is inserted, we may expect significant influence of the long-ranged, stress-field on the Li diffusivity. We tackle this problem by applying directly the hybrid QM-CL simulation method.

References

[1] e.g., S. Ogata, Y. Abe, N. Ohba, and R. Kobayashi, J. Appl. Phys, 108, 064313 (2010).