Yoshihide Yoshimoto

Institute for Solid State Physics, University of Tokyo
5-1-5 Kashiwa-no-ha Kashiwa-shi, Chiba, 2778581, Japan
Email: yosimoto@issp.u-tokyo.ac.jp

Session number 1

Bio

Y. Yoshimoto was awarded the doctoral degree in science at Department of Physics, Graduate School of Science, University of Tokyo, in 2000. The thesis work was supervised by Prof. M. Tsukada. After working as a research fellow of center of excellence program at Institute for Solid State Physics, University of Tokyo (ISSP), he became a research associate at ISSP. His scientific interests are in applications of first-principles method on surface science and in development of first-principles calculation methods. The works on developing the methods are on a plane-wave-based first-principles calculation program (an extended version of Tokyo ab-initio program package) and on a combination with multicanonical methods. He is also responsible for the operation of the super computer facility of ISSP, whose resource is served for researchers on materials science in Japan.

First-principles calculations combined with multicanonical ensemble method

The multicanonical ensemble [1,2] is a generalized ensemble whose statistical weight is not canonical one but (estimated) inverse of the density of states. Because of this property, the simulated system fluctuate widely from low energy states to high energy states. This enhanced fluctuation enables the system to overcome free energy barriers among low energy states quickly. The histories of the simulations are virtual, namely, not physical ones. Nevertheless, we can obtain thermodynamic quantity of any temperature from them by a method called reweighting. In this sense, these histories represent the whole thermodynamics of the systems as sets of thermodynamically relevant states.

Yoshimoto has focused on melting properties because it is a basic procedure for material synthesis and formation of objects (e.g. casting). For melting, multicanonical ensemble method has several merit compared to existing two-phase method (necessary system size is smaller) and thermodynamic integration method (no good reference system is required).

The paper will present his recent effort to apply multicanonical ensemble in first-principles calculations. This effort includes the *thermodynamic downfolding* of interatomic potentials that is a generation method of a model interatomic potential conserving the thermodynamics of the system simulated by a first-principles calculation to a maximum extent. In this method, the history of the multicanonical simulation is used as a measure for interatomic potentials. The presentation will pick up the melting of Si as a typical covalent crystal and MgO as a typical ionic crystal.

[1] B. A. Berg and T. Nuehaus, Phys. Lett. B 267, 249 (1991)
[2] J. Lee, Phys. Rev. Lett. 71, 211 (1993)
[3] Y. Yoshimoto, J. Chem. Phys. 125, 184103 (2006)