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First-principles calculation combined with multicanonical simulation YOSHIHIDE YOSHIMOTO, ISSP, University of Tokyo, 5-1-5 Kashiwa-no-ha, Kashiwa, 2778581, Japan — To tackle statistical complexities in condensed matters such as phase transitions of atomic structures with first-principles calculations, Yoshimoto have studied the combination of first-principles calculations and multicanonical methods. By the multicanonical methods, phase space of atomic coordinates can be explored efficiently. Among phase transitions, Yoshimoto focused crystal↔liquid transition because it is a basic procedure for material synthesis and formation of objects (casting). The talk will present his recent results : a direct (not a coexisting) simulation of the crystal↔liquid transition by a kind of two-component multicanonical ensemble, a *multi-order multi-thermal ensemble*, with an order parameter defined with structure factors that characterize the transition, and optimization of a model interatomic potential in terms of the ensemble from an accurate one called *thermodynamic downfolding* of a potential. These provide a principle to project a first-principles approach on a model-based approach conserving thermodynamic properties of multiple phases to a maximum extent. The talk will cover the successful applications of the method to the transition of Si and MgO. Ref: Y. Yoshimoto, J. Chem. Phys. 125, 184103 (2006)

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