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Crystal Structure Searching by Free Energy Surface Trekking: Application to Carbon above 1 TPa TAKAHIRO ISHIKAWA, Center for Quantum Science and Technology under Extreme Conditions, Osaka University, NAOSHI SUZUKI, Department of Pure and Applied Physics, Faculty of Engineering Science, Kansai University, KATSUYA SHIMIZU, Center for Quantum Science and Technology under Extreme Conditions, Osaka University — Crystal structure determination of materials under extreme conditions has been one of grand challenges in high-pressure materials science. In computer simulations, the crystal structure searching is carried out by exploring Gibbs free energy surface (GFES) at given pressures and temperatures. Here, we propose a new crystal structure searching technique named as free energy surface trekking (FEST). FEST is based on a very simple idea and consists of an ascent-run and a descent-run. In the ascent-run, the system is forced to ascend GFES from a starting local minimum by following the inversion of the driving force acting on the simulation cell. Then, the system descends it toward a neighboring local minimum by flipping the inverted force at the ridge of GFES. The details of GFES around the starting local minimum are more correctly obtained by more investigating different trekking routes. We have applied FEST to carbon at 1.2 TPa and at 300 K, and successfully obtained the transition from the cubic diamond phase to the previously predicted BC8 phase. In this transition, 3 cell-angles concurrently increase from 90° to 101° in the ascent-run and become 109° through the descent-run, in which the activation energy is approximately 0.17 Ry/atom.

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