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Thermodynamic Effects on Phase Stabilities and Structural Properties of TiO2 from the First-principles[1] YUTA AOKI, SUSUMU SAITO, Department of Physics, Tokyo Institute of Technology — Titanium dioxide (TiO2) is one of the most representative photocatalytic materials and much attention is focused on understanding and improvement of its photocatalytic activity. At the same time, TiO2 is known to be a highly polymorphic material and as many as eleven crystal phases have been identified so far. It is expected that TiO2 show various photocatalytic properties depending on crystal phases. However, relative stabilities of these identified phases are still controversial. In order to clarify the thermodynamic phase stabilities of TiO2, we obtain the free energies of its several representative phases, rutile, anatase, brookite, and TiO2-II within the framework of the density-functional theory using the pseudopotential method. We calculate both the static energy and the contribution of phonons to the free energy through the quasiharmonic approximation for each phase. It is found that treatment of semicore electrons in constructing the pseudopotential of the Ti atom significantly affects the relative phase stabilities. From the phase diagram obtained, we find that the anatase phase is the most stable at lower temperature and pressure. We also discuss the thermodynamic effects on structural properties such as thermal expansion.

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