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第一原理熱力学積分分子動力学法の開発と木星核の熱化学状態への応用
Insight into the thermochemical state of the Jovian core from ab initio thermodynamic integration MD

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The thermochemical state of the Jovian rocky core still remains unclear. Although the rocky components of the cores in gas giants are likely to be MgO, SiO_2 and Fe (Guillot, 1999), reported melting condition are still limited up to ~500-1500 GPa (Boates and Bonev, 2013; Millot *et al*., 2015; Bouchet *et al*., 2013), which are far lower than the Jovian core P,T condition (4 TPa and 20 kK) estimated based on the equations of state of gas materials determined by ab initio calculations (Nettelmann *et al*., 2012), primarily due to experimental difficulty. Thermochemical state (e.g., solid or liquid) of these materials might influence the tidal dissipation of planets and the mixing of the core and envelope. In order to clarify the phase equilibria, we have developed a new technique for calculating free energies of liquid and crystalline states based on the thermodynamic integration method (Frenkel and Smit, 2001) combined with the ab initio molecular dynamics method.

We obtained the following new findings: (1) calculated density of the MgO-SiO_2-Fe mixture is found highly consistent with the modeled Jovian core density, (2) although the melting temperatures of MgO and SiO_2 are higher than the modeled Jovian core temperature, the eutectic temperature is lower. These could serve for more detailed modeling of Jovian interior.
Keywords: ab initio calculation, thermodynamic integration method, Jovian core