Geodynamics Seminar

第375回ジオダイナミクスセミナー

Development of an *ab initio* calculation method for liquid free energy based on the thermodynamic integration

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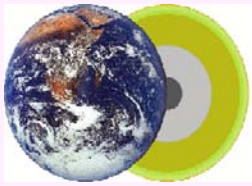
主催：愛媛大学地球深部ダイナミクス研究センター
日時：2/14（金）午後 4時30分～
場所：総合研究棟Ⅰ 4F 共通会議室



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Abstract

Gibbs free energies of phases are equal at a phase transition boundary. For crystalline solids, their free energies can be determined by the density functional perturbation theory and the quasi-harmonic approximation efficiently and accurately (e.g. Tsuchiya, 2003). However, it is difficult to determine free energies of liquids due to the difficulty on evaluating entropy in disorder structures. The thermodynamic integration (TI) method (Meijer *et al.*, 1990) based on statistical mechanics is known to be a powerful technique to calculate free energies of liquids since it directly accesses free energy without calculating entropy. In this study, a new method based on the TI technique has been developed combined with the ab initio molecular dynamics method and applied to determine melting points of major earth science materials.

In previous studies (e.g. Wilson and Militzer, 2012), liquid free energy was calculated by two-step TI, where the first step is an integration from an ideal gas system to a classical system, and the second step is an integration from a classical system to an ab initio system. In contrast, in this study, liquid free energy has been switched directly from an ideal gas system to an ab initio system.

The technique developed in this study is applied to determine the melting points of MgO and SiO_2. These are representative minerals and also major candidates of giant planetary constituents. Their melting temperatures are also well studied both experimentally and theoretically. Therefore, these oxides are suitable to be test materials for the present technique.

詳細は当センターホームページ： http://www.ehime-u.ac.jp/~grc/をご覧ください
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