The 491st Geodynamics Seminar

Application of ab initio simulations to element partitioning between silicate and metal

Dr. Taku Tsuchiya (Professor, GRC, ELSI-ES)

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Abstract

Earth's mantle and core interact with each other both physically and chemically. Conductive heat transport is for example important to consider their thermal coupling. On the other hand, one of key properties to study their chemical interaction is element partitioning between silicates and metals. In order to access this property within the computational mineral physics framework, free energy variations associated with compositional variations have to be evaluated. We achieve this by extending the thermodynamic integration method, which was successfully implemented to our ab initio molecular dynamics code to predict high-P,T melting curves. The technique has been applied so far to some geochemically interesting systems including K and noble gases.

EHIME UNIVERSITY GRC GEODYNAMICS RESEARCH CENTER

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Contact : Dr. Nishi (e-mail: nishi@sci.ehime-u.ac.jp)