

The 466th Geodynamics Seminar

Ab initio core model

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

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Abstract

Earth's inner core (329~364 GPa and 5000~6000 K) is thought to be composed of solid Fe-Ni alloy with some light elements. Thermoelasticity of iron and iron-light element alloys is therefore a key to interpreting seismological information of the inner core: density, seismic wave velocities, and their anisotropy. However, several studies reported that pure hcp iron has a shear modulus distinctly larger than that of the inner core (e.g., Mao et al., 1998; Vocadlo et al., 2009). This large Poisson ratio of the inner core is one of the remaining inexplicable features of the deep Earth, and some studies recently proposed this be explained by alloyed with light elements such as carbon (e.g., Chen et al., 2014) and hydrogen (e.g., Militzer, 2016). In this study, we perform ab initio molecular dynamics simulations of iron-light element (Si, C, and H) alloys and examine their seismic wave velocities and density to investigate the viability of iron alloys in the inner core.