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超高温高圧条件下における鉄、鉄-軽元素系の安定性及び弾性に関する第一原理計算 Ab initio study on the high-P,T phase relations and elasticity of iron and iron-light element systems

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The Earth's core is thought to consist of iron with some light elements (O, Si, S, C, etc). But the phase relations and physical properties of those systems are still underdetermined primarily due to experimental difficulty. The ab initio computation method is instead a strong technique to investigate materials under ultrahigh-pressure and temperature conditions. In this talk, I briefly summarize the current status of the computations of some core materials and discuss thermochemical properties of the Earth's core, including new findings related in particular to the large entropic effects likely expected at high core temperatures.

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Keywords: iron and iron-light elements system, high-pressure, stability and elasticity, ab initio method, Earth's core