

Structural and transport properties of liquid iron-light-element mixtures under outer core conditions

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It is widely believed that Earth's outer core consists of liquid iron (or liquid-nickel alloy) with light element (LE) impurities. For understanding magnetic and thermal behaviors of the Earth, it is required to explore electrical and thermal conductivities of liquid iron and influence of the light elements on these properties.

For this reason, we have investigated influences of light elements on transport properties of liquid iron under high pressure by using ab initio molecular dynamics simulations. We reported the structural and transport properties of liquid Fe-LE binary systems in connection with a microscopic structural properties. This times, in addition to binary systems, we have investigated transport properties of Fe-LE ternary systems. To provide further details of the effects of light-element, we discuss structural and transport properties of liquid Fe alloys in terms of the type and amount of light elements.

Keywords: liquid iron alloy, ab initio molecular dynamics simulation, transport properties, high pressure properties