Water partitioning between liquid metal and molten silicate under high pressure and temperature

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Metal/silicate water partitioning under high pressure is important to understand the water circulation in Earth's deep interior. Several srudies have therefore been conducted both experimentally and theoretically. However, primarily due to the technical difficulty in quantitative analyses of hydrogen, the reported experimental resuts scatter largely. Recent theoretical studies, on the other hand, suggest a siderophile behavior of hydrogen under high pressure, but those assume a simple molecular exchange reaction only and the stability of an experimentally suggested redox reaction is yet to be investigated. Therefore, the nature of metal/silicate partition reaction of water under high pressure remains largely unclear. In this study, we perform the ab initio free energy calculations based on the density functional theory and the thermodynamic integration method and predict reaction energy related to the high-pressure water partitioning between liquid iron and silicate melt with several different compositions considering both molecular exchange and redox reactions.

Keywords: Ab initio free energy calculations, Thermodynamic integration method, Metal/silicate water partitioning

