First-principles prediction of hydrogen partitioning between the core and mantle

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Some recent studies have reported high-P,T hydrous minerals which are stable at the core mantle boundary (CMB) pressure (Sano et al., 2008; Ohhira et al., 2016; Nishi et al., 2017). In order to elucidate the water circulation in the Earth's interior, experiments on the reaction between iron and hydrous minerals or water were also conducted (Iizuka-Oku et al., 2016; Mao et al., 2018; Clesi et al., 2018). However, the partition of hydrogen reported is different in different studies. In this study, we try estimating hydrogen partitioning between molten silicate and liquid iron under the CMB conditions based on the first principles calculation method combined with thermodynamic integration similar to our previous study (Xiong et al., 2018). Here, we assume following the exchange reaction of water between liquid iron and molten silicate is expressed as follows
(16MgSiO3+H2O) + 50Fe ⇔16MgSiO3 + (50Fe+H2O)
as a first example with ensuring the charge neutrality. Here, reaction free energy is calculated by the thermodynamic integration molecular dynamics method (Taniuchi & Tsuchiya, 2018). In the moment, simulations suggest that water prefer liquid iron. Now, additional computations are ongoing for improving numerical accuracy. The mechanism dissolving water into liquid iron is also investigated.

