Core-mantle differentiation in a hydrous magma ocean

HAIYANG LUO AND JIE DENG

Princeton University

Presenting Author: haiyang.luo@princeton.edu

Water's role in planetary composition is profound, with recent research suggesting its involvement in crucial chemical reactions with silicon and/or iron within magma oceans during core-mantle differentiation. However, accurately quantifying the effect of water on metal-silicate reactions under extreme conditions of high temperature and pressure poses significant challenges in both experimental and computational domains. To address this, we first train machine learning potentials of ab initio quality for the H-O-Mg-Si-Fe system and then conduct large-scale molecular dynamics simulations of metal-silicate coexistence to investigate the water content dependence of the metal-silicate partitioning behavior of these elements. Integrating our findings with experimental data on metal-silicate partitioning, we construct a thermodynamic model capable of describing the partitioning of H, O, Mg, Si, and Fe in a wide temperature, pressure, and compositional space. We find that water affects the metal-silicate partitioning behavior of these elements to different extents. This offers us a chance to constrain Earth's initial water content during the magma ocean stage and Earth's core and mantle compositions (e.g., Mg/Si ratio) simultaneously. Our results are also fundamental for interior modelling of water-rich exoplanets and have direct consequences on inferred water mass budgets from mass-radius data of exoplanets.