Machine learning silicate systems at extreme conditions

Jie DENG
(University of California, Los Angeles)

Silicates are the major building blocks of terrestrial planets and exoplanets. The thermochemical states of silicates and their phase transitions, to a large extent, dictate a planet's evolution. Experiments that simulate extreme planetary conditions, for example, the Moon-forming giant impact or super-Earth interiors, are difficult. *Ab initio* atomistic simulations, although may reach a wide pressure and temperature range, are limited to small systems that consist of a few hundreds of atoms due to the large computational costs. However, atomistic modeling on processes such as melting, crystallization, vaporization, condensation, deformation, and miscibility usually requires large systems. Recently, the emerging machine learning molecular dynamics simulations offer an unprecedented opportunity to solve this problem. Machine learning molecular dynamics simulations employ potential energy surfaces learned from quantum mechanical calculations, which tremendously accelerates atomistic modeling and enables simulating systems up to millions of atoms. In this talk, I will present our recent simulation results of silicates using machine learning potentials.

Bio

Jie earned his Ph.D. degree in geophysics at Yale University in 2019 under the supervision of Kanani Lee. He studied the melting and dynamics of Earth's deep interior at extreme conditions using both high-pressure experiments and the density functional theory, for which he received the Graduate Research Award in Study of Earth's Deep Interior of American Geophysical Union 2018 Fall meeting. After that he joined the Department of Earth, Planetary, and Space Sciences at UCLA as a post-doctoral scholar working with Lars Stixrude. He will join the faculty of the Princeton Geosciences Department as an assistant professor in 2022.