

# **Bonding and transport dynamics and mixing mechanism of liquid Fe-light elements under the Earth's outer core conditions**

JIANWEI WANG AND SAJIN SATYAL

Louisiana State University

Presenting Author: [jianwei@lsu.edu](mailto:jianwei@lsu.edu)

Properties of Fe-alloys under Earth's core conditions are essential for understanding the core composition, thermal state, dynamics, and evolution. The effect of light elements (H, C, O, Si, and S) on density and seismic velocity profiles provides direct clues to constrain their presence in the core. Each light element has its unique effect along the outer core adiabat, controlled by its nature and how it mixes with Fe. This study focuses on the electronic structure and dynamics of chemical bonding, mixing mechanisms, and diffusive properties. First-principles molecular dynamics was employed to simulate five binary systems (Fe-H, C, O, Si, and S) at the temperature and pressure conditions (4050-5530 K and 135-330 GPa) along the outer core adiabat. The results show that the bonding is complicated, depending on the light element and conditions and how it is incorporated into the liquid. Electron localization function and density of states suggest that the electrons around Fe are highly delocalized, reflecting the metallic nature of Fe. There is a significant but decreasing electron localization for H, O, C, S, and Si, suggesting H and O have a higher ionic nature than C and S. The latter two show significant electron sharing with Fe, suggesting a covalent nature of the interactions. Si shows the highest metallic nature among the light elements. The bonding characteristics are correlated to the bonding dynamics as measured by the mean bonding lifetime and self-diffusion coefficient. Local structure analysis shows interstitial mixing of H atoms in both tetrahedral and octahedral sites in the approximately close packed structure, with a pathway for diffusion through the polyhedral faces. Rest light elements demonstrate a replacement mixing mechanism with different interstitial occupancies. Both C and O have a significant octahedral interstitial occupancy and a minor tetrahedral occupancy. S only has a minor octahedral occupancy. Si is mostly replacement mixing. Activation energy and volume for bonding dynamics, diffusion, and viscosity were calculated and are correlated to the chemical bonding and mixing mechanism of the elements. The results provide a foundation for constraining the earth's core composition and understating the light elements in the core.