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Molecular Hydrogen Behavior in Deep Mantle Minerals

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Volatile hydrogen, as the primary carrier of water in the mantle, plays a crucial role in Earth's climate and habitability. Recent studies have revealed that hydrogen in the mantle does not exist solely in the form of hydrates or hydroxyl groups (OH). Particularly under the highly reduced conditions of early Earth or terrestrial planets, hydrogen may stably exist in mantle minerals in the form of molecular hydrogen (H_2)[1]. Grain boundaries(GBs), as structural defects or interfaces in materials, often exhibit markedly different physicochemical properties compared to the bulk, potentially providing unique pathways for hydrogen storage and migration. Current in-depth studies on hydrogen dissolution and diffusion in minerals predominantly focus on the properties of the mineral bulk[2], with less attention paid to GBs regions. However, relying solely on lattice diffusion models cannot adequately explain the differences in diffusion between H_2 and other occurrence mechanisms in mantle minerals.

This study combines first-principles calculations and machine learning force fields to systematically investigate the diffusion behavior of H_2 in the bulk and GBs of olivine and periclase, with a particular focus on the differences between lattice diffusion and GBs diffusion. The results demonstrate that H_2 can stably exist in the bulk and GBs of olivine and periclase under high-pressure and high-temperature conditions, especially in low oxygen fugacity environments, which is consistent with the reduced conditions of early Earth or terrestrial planets. Furthermore, the diffusion rate of H_2 in GBs is significantly higher than in the bulk phase, with GBs diffusion coefficients approximately two orders of magnitude larger than those in the bulk. This indicates that GBs provide a more favorable environment for hydrogen migration and may serve as critical pathways for the transport of H_2 under upper mantle conditions.

These findings provides new insights into understanding the deep-Earth water cycle and its evolution, and also offers important references for research on the deep water cycles of early Earth and other terrestrial planets.