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Helium adsorption on the (001) plane of MgO: A possible candidate in the lower mantle to contain noble gases

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Noble gases (mostly He and Ar) are used as tracers to investigate the geochemical evolution of the mantle and atmosphere due to their inertness and volatility. Among the Helium isotopes, ^{3}He is the primordial one that was included during Earth's accretion, while ^{4}He is the decay product of U and Th. Even though the majority of ^{3}He has been degassed, the strong affinity of Ca-perovskite towards U and Th leads to the formation of ^{4}He in the lower mantle [1]. Additionally, during the subduction, a small fraction of ^{4}He manages to reach the mantle, which can significantly affect the helium concentration of the Earth's interior. The lower mantle mineral phases that may contain He, however, remain mostly unexplored.

Zhang et al. in 2021 proposed that helium can form compounds with Fe under the p-T conditions of CMB [2]. A recent study identified the ability of aragonite to accommodate He up to 40 GPa [3]. However, the mineral phases in the lower mantle that can potentially hold He are not explored in detail. Due to its inertness, it is difficult to incorporate the He into the lower mantle minerals via substitution. Adsorption of elements into mineral phases has recently received significant interest in the scientific world. Therefore, we can consider adsorption to be an effective mechanism for adding He to the lower mantle minerals. In the present study, we adsorb helium atoms on the (001) crystallographic plane of periclase (MgO), which is one of the abundant mineral phases in the lower mantle. The structural stability and the adsorption energy are examined till 135 GPa (CMB pressure condition) by employing DFT calculations. A negative adsorption energy indicates the structural stability of the aforesaid phase and the mechanical and dynamical stability will be investigated further.

References:

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