# Adsorption of Helium and Argon on the (001) Surface of Periclase: A First-Principles Study

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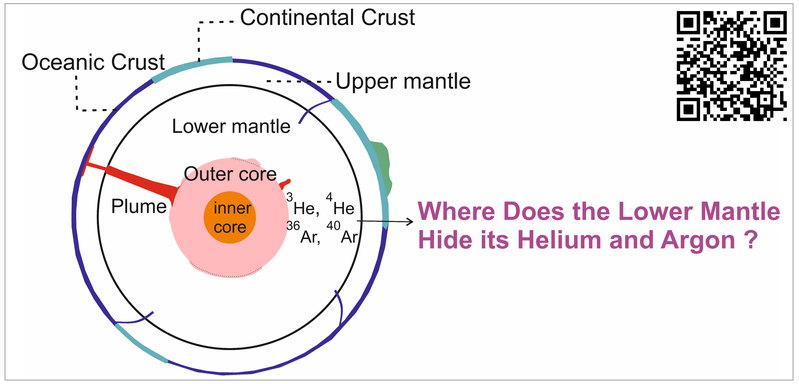



## Introduction

- Noble gases are vital tracers for the geochemical evolution of Earth's mantle and atmosphere (1).
- Helium and argon isotopes (primordial $^{3}$He and $^{36}$Ar; radiogenic $^{4}$He and $^{40}$Ar) in Ocean Island Basalts (OIB) and Mid-Ocean Ridge Basalts (MORB) confirm deep-seated mantle reservoirs (2).
- While multiple retention mechanisms exist, experimentally observing how lighter gases (He, Ar) are incorporated into the lower mantle minerals at extreme pressure remains challenging (1).
- This research explores the incorporation of Helium and Argon within periclase (MgO), a primary lower mantle mineral, under pressure conditions reaching the Core-Mantle Boundary (CMB).

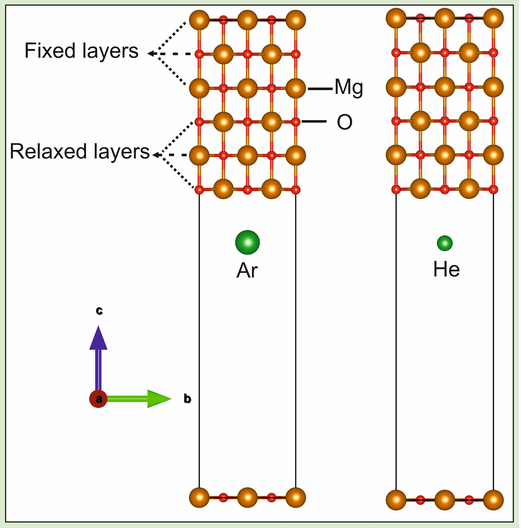
## Structural analysis

- **Substrate Geometry:** 6 periodic layers of MgO (001) with a total thickness of 10.6 Å.
- **Supercell Construction:** Expanded to a 2×2×1 supercell for enhanced lateral dimensions.
- **Vacuum added:** 20 Å .
- **Selective Dynamics:**

✓ Bottom 3 layers: Fixed to represent the stable bulk crystal.
✓ Top 3 layers: Fully relaxed to accommodate gas interaction.

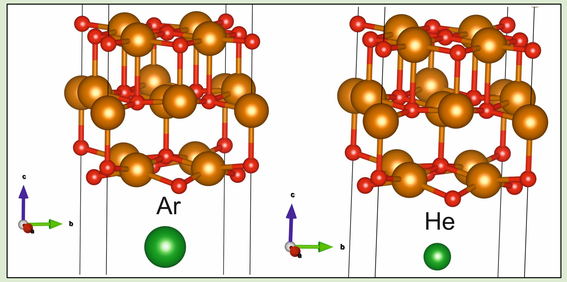
- **Adsorption Sites:** He and Ar atoms positioned directly above the central Oxygen (O) atoms on the surface.

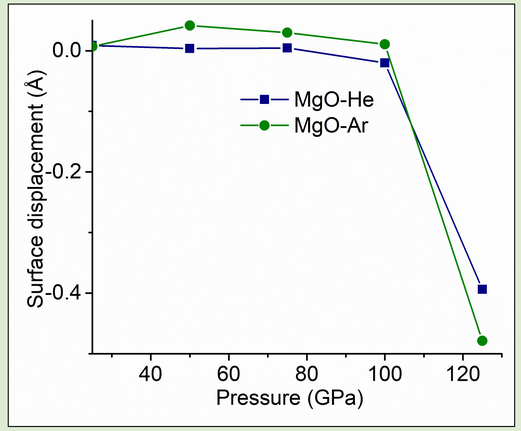
## Results and discussions




Optimized structures of Ar and He adsorbed on the MgO (001) plane at 0 GPa.
Adsorption causes no significant distortion of the surface layers.

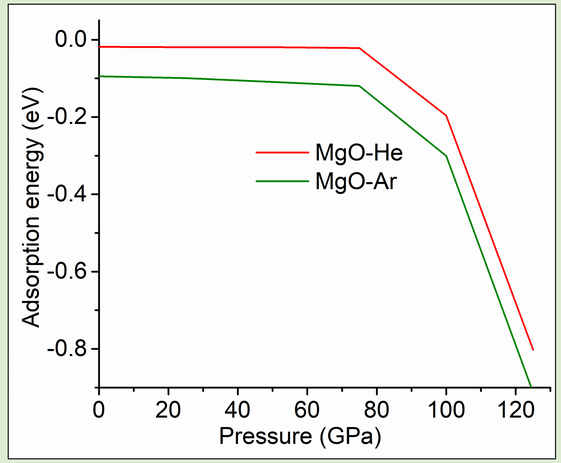
- At 100 GPa, the drastic reduction in interatomic distance between the noble gases (He, Ar) and surface oxygen ions triggers strong Pauli repulsion. This electronic overlap necessitates a significant structural relaxation, manifesting as the observed surface distortion.
- Surface distortion may also be influenced by a potential pressure-induced phase transition in the MgO lattice. Ongoing investigations into the mechanical and dynamic stabilities (e.g., phonon dispersions) will further elucidate the fundamental drivers of this structural instability.




- The displacement of the oxygen atom above which the adsorption takes place shows an average decrease with an increase in pressure.
- After 75 GPa, there is a sudden decrease in the displacement, indicating the surface distortion.

- The adsorption energy is found to be inversely correlated with the pressure.
- The adsorption energy of argon is found to be less than that of helium in all pressure conditions.
- There is a drastic decrease in the adsorption energy after 75 GPa, indicating the accelerated reactivity of noble gases under extreme conditions.




## Conclusions

- Adsorption acts as an effective method in incorporating noble gases within periclase under high-pressure conditions.
- The surface layers of the periclase were found to be distorted under extreme pressure conditions.
- The adsorption energy becomes more negative with an increase in pressure.
- The retention of argon in the Earth's interior is more than that of helium

## References

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## Methodology

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