

A possible reservoir for primordial helium in the lowermost mantle

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There is compelling geochemical evidence for primordial helium trapped in Earth's lower mantle, but the origin and nature of the helium source remain elusive due to scarce knowledge on viable helium-bearing compounds that are extremely rare. Here we explore materials physics underlying this prominent challenge. Our structure searches in conjunction with first-principles energetic and thermodynamic calculations uncover a remarkable helium-bearing compound FeO_2He at high pressure-temperature conditions relevant to the core-mantle boundary. Calculated sound velocities consistent with seismic data validate FeO_2He as a feasible constituent in ultralow velocity zones at the lowermost mantle. These mutually corroborating findings establish the first and hitherto only helium-bearing compound viable at pertinent geophysical conditions, thus providing vital physics mechanisms and materials insights for elucidating the enigmatic helium reservoir in deep Earth.