

Abstract Submitted
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Searching for viable transition paths of pressure driven phase transition in solid xenon: First-principle study¹ EUNJA KIM, Department of Physics and High Pressure Science and Engineering Center, University of Nevada, Las Vegas, Nevada 89154 — Pressure induced structural transformation in solid xenon has been investigated using a first-principles calculation. Enthalpy calculation confirms that the fcc-to-hcp transformation begins around 5 GPa and finishes up around 70 GPa. We propose two transformation pathways in solid xenon such as a stacking disorder growth pathway at low pressure (Path-I) and an orthorhombic distortion pathway followed by atomic rearrangements at high pressure (Path-II). Delicate interplay of enthalpy and energy barrier will be discussed to explain the underlying mechanism of how solid xenon selects the proper transformation pathways under pressure.

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