A Comparative Study of GaAsO₄ Polymorphs: ab initio Calculations on High-pressure Forms

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Dedicated to Professor Gérard Demazeau on the occasion of his 65th birthday

First-principles calculations were performed to compare the relative stability and high-pressure behavior of four different GaAsO₄ polymorphs: the ordinary-pressure phase (berlinite, α-quartz-like) and three high-pressure phases: the β-VCrO₄-like, the rutile-like and a new hexagonal form, recently discovered and related to rutile.

Key words: Gallium Arsenate, High-pressure Polymorphs, ab initio Calculations