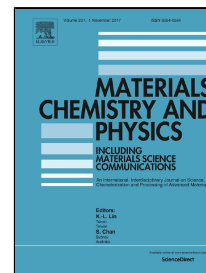


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High-pressure phase transition and thermodynamic properties from first-principles calculations: Application to cubic copper iodide



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1. Structural, elastic, and thermodynamic properties of CuI in high-pressure rocksalt phase are investigated systematically.
2. Some interesting thermodynamic parameters are successfully obtained based on the quasi-harmonic Debye model.
3. In the whole research the pressure and temperature up to 100 GPa and 800 K, respectively.

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