

Abstract Submitted
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First-principles study of high-pressure phase transitions in Si_3N_4 ¹

BIN XU, JIANJUN DONG, Physics Department, Auburn University, HAROLD STOKES, Brigham Young University, DORIAN HATCH, Brigham Young University — We have performed a systematic theoretical study of phase transitions in Si_3N_4 at high-pressure. We calculated the Gibbs free energies of the ground state β phase and the high-pressure γ phase at various temperatures and pressures based on the first-principles density functional theory and the statistical quasi-harmonic theory. The thermal equations of state and the Clapeyron slope of the β -to- γ transition at high-pressure are determined and compared with available experimental data. In addition to the recently discovered high-pressure γ -phase, we predict a new high-pressure phase of hexagonal symmetry. This new high-pressure phase is likely to exist metastably at the high pressure *and room temperature*, and it is associated with a non \AA -point soft phonon distortion. The structural and elastic properties and the stability condition of this predicted metastable high-pressure phase will be discussed.

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