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Density Functional Theory Investigation of Sodium Azide at High Pressure BRAD STEELE, AARON LANDERVILLE, IVAN OLEYNIK, University of South Florida — Sodium azide is intriguing because it could potentially be used as a precursor to a high-nitrogen energetic material. Furthermore, recent absorption and Raman spectroscopic results have shown that novel nitrogen structures may indeed be attainable from sodium azide. First-principles density functional theory calculations were performed to characterize possible novel crystalline structures of sodium azide including their atomic structure, vibrational properties, Raman spectra, and equation of state up to 90 GPa. Calculated Raman peaks and intensities show good agreement with experiment.

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