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Nitrogen-rich mixtures for high-energy density applications¹

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Nitrogen transforms from molecular to polymeric phase at high pressure. Polymeric nitrogen is one of the most studied candidates for high energy density materials. There is an interesting question of whether introducing small amount of impurities can alter the polymerization to lower pressures and lead to enhanced metastability. To address this, we have used first-principles density functional theory to study the electronic, structural, and dynamical properties of nitrogen-rich mixtures. We have identified several solid phases for different nitrogen concentrations and investigated the thermodynamic stability of solid and liquid mixtures with respect to their pure components.

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