

# THERMODYNAMICS OF NONMOLECULAR NITROGEN AT HIGH TEMPERATURES AND DENSITIES

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Experimental studies (both shock-wave and diamond-anvil) reveal unusual behavior of Hugoniot and the melting curve of highly compressed nitrogen at megabar pressures which is interpreted as transformation of molecular nitrogen to nonmolecular (atomic or polymeric) phases. Ab-initio calculations predict polymorphism of nitrogen at high pressure and first-order solid-solid and liquid-liquid phase transitions in compressed nitrogen. In this work we demonstrate the possibility to represent interactions of nitrogen on atomistic level and calculate thermodynamic properties of its nonmolecular phases using conventional Monte Carlo simulations.