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Polymerization of sodium-doped liquid nitrogen under pressure¹ STANIMIR BONEV, Lawrence Livermore Natl Lab, MARC CORMIER, Lawrence Livermore Natl Lab, Dalhousie University — Using first-principles theory, we have investigated the possibility of reducing the polymerization pressure of N through impurity doping. A description of structural and electronic properties leading to an understanding of the effect of Na-doping on the polymerization phase transition will be presented. We show that it develops in three distinct stages, commences at much lower pressure compared to the pure N system even with a small Na concentration, and there are qualitative changes in its evolution beyond a certain Na concentration.

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