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Ab-initio Based Simulations High-Pressure Phases of Nitrogen
FEDERICO ZAHARIEV, ANGUANG HU, JAMES HOOPER, TOM WOO, University of Western Ontario, Canada, FAN ZHANG, Defence R&D Canada-Suffield, Canada — The existence of cubic-gauche polymeric form of nitrogen was first predicted theoretically in 1992 and recently confirmed experimentally, further increasing the interest in polynitrogen as a potential high energy density material. We present three new polymeric phases of nitrogen under pressure: 3D chaired six-ring network, 2D boated six-ring layers, 1D chaired six-ring chains. The 3D chaired six-ring network has an enthalpy intermediate between those of black-phosphorus and cubic gauche up to 120GPa. Our simulations provide an insight into the phase transitions of the new metastable phases.

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