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Surface Stability of Polymeric Phases of Nitrogen JAMES HOOPER, FEDERICO ZAHARIEV, TOM WOO, University of Western Ontario, Canada, FAN ZHANG, Defense R&D Canada-Suffield — The polymeric phases of nitrogen have been actively studied, including the prediction of cubic gauche that has recently been observed experimentally under conditions of high pressure. The stability and electronic properties at their surfaces are important for the practical application of these materials. We present a theoretical and computational study of the surface of cubic gauche with or without dopants capping the dangling bonds. Use of various capping groups does stabilize the surface. This study uses ab-initio density functional simulations.

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