

Abstract Submitted
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Theoretical precursors to polymeric nitrogen RAZVAN CARACAS, Bayerisches Geoinstitut, RUSSELL J. HEMLEY, Carnegie Institution of Washington — We predict the existence of new structures of nitrogen based on new observations in analog systems from first-principles density-functional calculations. A series of structures was examined. A structure with orthorhombic symmetry is stable relative to the ϵ and *cubic gauche* phases in LDA, whereas GGA shows the ϵ and the new orthorhombic structure are energetically competitive. This structure is dynamically stable at least from ambient pressure to 90 GPa and thus may be observed as a stable or metastable polynitrogen phase prior to the transition to the atomic phases of nitrogen.

Razvan Caracas
Bayerisches Geoinstitut

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