

Abstract Submitted
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First-order liquid-liquid phase transition in compressed nitrogen¹

BRIAN BOATES, STANIMIR BONEV — We present results of first-principles molecular dynamics simulations, which provide evidence for the existence of a first-order liquid-liquid phase transition in compressed nitrogen [1]. The transition is from a molecular to a polymeric liquid. It is characterized by a discontinuous loss of molecular stability followed, upon further compression, by gradual transformation until the local order of the liquid becomes similar to that of cg-N. We have computed the phase boundary of the liquid-liquid transition to be first-order between 2000 and 4000 K and determined that above 4000 K it becomes continuous. Comparison with measurements and suggestions for experimental confirmation of our predictions will be discussed as well. [1] B. Boates and S.A. Bonev, submitted.

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