Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

A systematic search method for finding new high-pressure phases of polymeric nitrogen SERGEY DUDIY, FEDERICO ZAHARIEV, JAMES HOOPER, Department of Chemistry, University of Ottawa, Ottawa, Ontario, K1N 6N5, Canada, FAN ZHANG, Defense Research and Development Canada - Suffield, PO Box 4000, Medicine Hat, Alberta, T1A 8K6, Canada, TOM WOO, Department of Chemistry, University of Ottawa — A recent discovery of single-bonded polymeric form of nitrogen in diamond anvil cell high pressure experiments [Nature Mat. **3**, 558 (2004)] opens a new promising direction in the development of high energy density materials. Besides the cubic gauche phase of polynitrogen stabilized in experiment, other yet unidentified metastable phases could emerge under certain experimental conditions. We present a systematic search method for finding metastable phases of single bonded nitrogen based on a set of Peierls distortions of a given reference structure. Using the most basic reference structure, a simple cubic unit cell, our approach not only reproduces all the single-bonded nitrogen phases reported so far, but also reveals many new metastable structures with promising properties. The equations of state of the structures calculated at the first-principles level are studied over a broad range of pressures up to 300 GPa. The stability of the structures is analyzed using directly calculated phonon spectra. This approach can be extended using more complex reference structures and relaxing the constraint of a pure single bonded phase.

Tom Woo
University of Ottawa

Date submitted: 30 Nov 2005 Electronic form version 1.4