Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

On calculating the equilibrium structure of molecular crystals
ANN E. MATTSSON, RYAN R. WIXOM, THOMAS R. MATTSSON, Sandia National Laboratories, Albuquerque, NM 87185 — The difficulty of calculating the ambient properties of molecular crystals, such as the explosive PETN, has long hampered much needed computational investigations of these materials. One reason for the shortcomings is that the exchange-correlation functionals available for Density Functional Theory (DFT) based calculations do not correctly describe the weak intermolecular van der Waals' forces present in molecular crystals. However, this weak interaction also poses other challenges for the computational schemes used. We will discuss these issues in the context of calculations of lattice constants and structure of PETN with a number of different functionals, and also discuss if these limitations can be circumvented for studies at non-ambient conditions. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Ann E. Mattsson
Sandia National Laboratories, Albuquerque, NM 87185

Date submitted: 17 Dec 2009 Electronic form version 1.4