Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Dispersion Interactions in High-Density Molecular Crystals PETER CSERNICA, RAHUL MAITRA, ROBERT DISTASIO , Cornell University — Dispersion interactions are ubiquitous quantum mechanical phenomena arising from correlated electron density fluctuations in molecules and materials. As a key component of non-bonded interactions, dispersion forces play a critical role in determining the structure and stability of molecular crystals. Due to the relative intermolecular separation in high-density molecular crystals, an accurate description of these non-bonded interactions requires the inclusion of terms beyond the asymptotic induced-dipole–induced-dipole (C_6/R^6) contribution. In this work, we have developed a first principles based approach within the framework of Density Functional Theory (i.e., that only depends on the charge density $n(\mathbf{r})$) for capturing the higher-order induced multipolar contributions to the correlation energy. As a first application of this method, we have investigated the structure and stability of the high-density ice molecular crystal polymorphs at the ice VI—ice VII—ice VIII triple point (278K, 2.1GPa) using *ab-initio* molecular dynamics in the isobaric-isothermal (NpT) ensemble.

Peter Csernica
Cornell University

Date submitted: 06 Nov 2015 Electronic form version 1.4