

Abstract Submitted  
for the MAR12 Meeting of  
The American Physical Society

**The Role of Many-Body Dispersion Interactions in Molecular Crystal Polymorphism** LESLIE LEISEROWITZ, Weizmann Institute of Science, Rehovoth, Israel, NOA MAROM, Institute for Computational Engineering and Sciences, The University of Texas at Austin, ROBERT A. DISTASIO, JR., Department of Chemistry, Princeton University, NJ, VIKTOR ATALLA, SERGEY LEVCHENKO, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, SERGEY KAPISHNIKOV, Weizmann Institute of Science, Rehovoth, Israel, JAMES R. CHELIKOWSKY, Institute for Computational Engineering and Sciences, The University of Texas at Austin, ALEXANDRE TKATCHENKO, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — Molecular crystals often have several polymorphs that are close in energy (few meV per molecule), but possess very different physical and chemical properties. Treating polymorphism from first principles has been a long standing problem because conventional density-functional theory (DFT) lacks a proper description of long-range dispersion interactions that govern the structure and energetics of molecular crystals. Here we assess the effect of the many-body dispersion (MBD) energy on the structure and relative energies of the polymorphs of benchmark molecular crystals: glycine, alanine, and para-diiodobenzene. This is accomplished by using the recently developed first-principles DFT+MBD method [A. Tkatchenko, R.A. DiStasio Jr., R. Car, M. Scheffler, submitted], based on the earlier Tkatchenko-Scheffler (TS) dispersion correction [PRL 102, 073005 (2009)]. We show that the non-additive MBD energy plays a crucial role in making qualitatively and quantitatively accurate predictions for the structure and relative energies of polymorphs.

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Date submitted: 28 Nov 2011

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