

Abstract Submitted  
for the MAR12 Meeting of  
The American Physical Society

**Higher-order van der Waals coefficients from static multipole polarizability**<sup>1</sup> JIANMIN TAO, JOHN PERDEW, ADRIENN RUZSINSZKY, Tulane University — van der Waals interaction is a long-range nonlocal correlation arising from instantaneous charge fluctuations on each fragment. Though very weak, it considerably affects the properties of molecules and solids. Evaluation of van der Waals coefficients is of strong current interest. In this work, we have derived a general expression for these coefficients in terms of static multipole polarizability only. Applications of the present theory to atom as well as molecular pair interactions have been made.

<sup>1</sup>This material is based upon work supported by the National Science Foundation under the NSF Cooperative Agreement No. EPS-1003897 with additional support from the Louisiana Board of Regents.

Jianmin Tao  
Tulane University

Date submitted: 08 Nov 2011

Electronic form version 1.4