Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Modeling graphene interactions beyond pairwise additivity[1]
JOHN DOBSON, TIM GOULD, Griffith University — Dispersion (van der Waals) interactions between graphenic systems are commonly modeled by summing energy contributions between pairs of atoms or '"elements". This pairwise assumption is now known to be inaccurate for such highly polarizable, highly anisotropic systems [1-5]. Many-electron correlation theories of RPA type [6] are more accurate, but are computationally intensive. Here we present a relatively simple type of model, based on long-wavelength RPA dielectric function data for stretched bulk graphite, that captures the non-additive physics. [1] J. F. Dobson, A. White, and A. Rubio, Phys. Rev. Lett. 96, 073201 (2006) [2] H. Y. Kim, J. O. Sofo, D. Velegol, M. W. Cole, and A. A. Lucas, J. Chem. Phys. 124, 074504 (2006) [3] A. White and J. F. Dobson, Phys. Rev. B 77, 075436 (2008) [4] A. J. Misquitta, J. Spencer, A. J. Stone, and A. Alavi, Phys. Rev. B 82, 075312 (2010) [5] R.-F. Liu, J. G. Angyan and J. F. Dobson, J. Chem. Phys. 134, 114106 (2011) [6] S. Lebegue, J. Harl, T. Gould, J. G. Angyan, G. Kresse, and J. F. Dobson, Phys. Rev Lett. 105, 196401 (2010)

[1]Work supported by the Australian Research Council

John Dobson
Griffith University

Date submitted: 09 Nov 2012 Electronic form version 1.4