Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Adiabatic Connection and Virial Theorem for Ensemble Density Functional Theory AURORA PRIBRAM-JONES, Department of Chemistry, University of California, Irvine, CA 92697, ZENG-HUI YANG, CARSTEN ULLRICH, Department of Physics and Astronomy, University of Missouri, Columbia, MO 65211, RICHARD NEEDS, Theory of Condensed Matter Group, Cavendish Laboratory, University of Cambridge, Cambridge CB3 0HE, United Kingdom, KIERON BURKE, Departments of Physics and Chemistry, University of California, Irvine, CA 92697 — Ensemble density functional theory (DFT) establishes a natural framework for thermal DFT and provides excited state information inaccessible through other DFT methods. However, development of better exchange-correlation approximations is needed for this theory to be of practical use [1]. In this talk, the adiabatic connection [2] and virial theorem for ensemble DFT will be presented. In particular, their relation to exact ensemble DFT calculations, dependence on ensemble weights, and a new method for extracting exact ensemble exchange-correlation potentials will be explored. [1] Gidopoulos, N. I. and Papaconstantinou, P. G. and Gross, E. K. U. *Phys. Rev. Lett.*, **88**, 033003 (2002). [2] Nagy, A. *Int. J. Quant. Chem.*, **56**, 225 – 228 (1995).

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Date submitted: 15 Nov 2013 Electronic form version 1.4