Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Finding Partition Potentials JONATHAN NAFZIGER, Department of Physics, Purdue University, MORREL COHEN, Department of Physics and Astronomy, Rutgers University and Department of Chemistry, Princeton UniVersity, ADAM WASSERMAN, Department of Chemistry, Purdue University — Partition Density Functional Theory is a formally exact approach to partitioning molecules into fragments via functional minimization and constraints on fragment densities. Cohen and Car proposed a Dynamical Optimization Algorithm for Partition Theory inspired by the Car-Parrinello Method of electronic structure [1]. We modify this algorithm to incorporate a reference HOMO wave-function calculation as a guide to obtain the partition potential, a global quantity arising as the Lagrange multiplier that guarantees satisfaction of the density constraint. We report on the implementation of this procedure for one-dimensional systems, and possible implications for linear-scaling electronic-structure calculations.

[1] M. H. Cohen, and R. Car, J. Phys. Chem. A 2008, 112, 571-575

Jonathan Nafziger
Purdue University

Date submitted: 16 Nov 2011 Electronic form version 1.4