Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Simple Illustration of Partition Theory ADAM WASSERMAN, Department of Chemistry - Purdue University, MORREL COHEN, Department of Physics - Rutgers University, and Department of Chemistry - Princeton University, KIERON BURKE, Department of Chemistry - UC-Irvine, ROBERTO CAR, Department of Chemistry - Princeton University — In Partition Theory (PT) [M.H. Cohen and A. Wasserman, J.Phys. Chem. A 2007, 111, 2229], the density of a system is decomposed exactly into a superposition of the densities of its parts through the introduction of a common *partition potential* acting on each of the parts as if they were isolated. In this talk we illustrate PT on a simple one-dimensional model of a heteronuclear diatomic molecule. We show that a sharp definition for the charge of the fragments emerges from PT, and that the ensuing population analysis can be used to study how charge redistributes during dissociation. By studying the preservation of the shapes of the parts as different parameters of the model are varied, we address the issue of transferability of the parts. We find good transferability within the chemically meaningful parameter regime, raising hopes that PT will prove useful in chemical applications.

Adam Wasserman
Purdue University

Date submitted: 21 Nov 2008 Electronic form version 1.4