Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Prediction of Born-Oppenheimer Interatomic Forces Using Orbital-Free Density Functional Theory with Approximate Kinetic Energy Functionals[1] S.B. TRICKEY, V.V. KARASIEV, FRANK E. HARRIS[2], Quantum Theory Project and Department of Physics, U. of Florida — Rapid calculation of Born-Oppenheimer forces is essential for driving the so called quantum region of a multi-scale molecular dynamics (MD) simulation. The orbital-free (OF) DFT approach is appealing but has proven difficult to implement because of the challenge of constructing reliable orbital-free approximations to the kinetic energy functional. To be maximally useful for multi-scale simulations, an OF-KE functional must be local (i.e. one-point). In the face of these difficulties, we demonstrate that there is a way forward. By requiring only that the approximate functional deliver high-quality forces, by exploiting the "conjointness" hypothesis of Lee, Lee, and Parr, by enforcing a basic positivity constraint, and by parameterizing to a carefully selected, small set of molecules we are able to generate a OF-KE functional that does a good job of describing various $H_qSi_mO_n$ clusters as well as CO and H_2O (providing encouraging evidence of transferability).

[1]Supported in part by U.S. NSF ITR Grant DMR-0218957
[2]also Dept. of Physics, U. of Utah

Sam Trickey
University of Florida

Date submitted: 21 Nov 2005 Electronic form version 1.4