Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Constraint-based, Single-point Approximate Kinetic Energy Functionals[1] FRANK E. HARRIS, Physics, University of Utah, V. V. KARASIEV, Instituto Venezolano de Investigaciones Cientificas, R. S. JONES, Loyola College of Maryland, S. B. TRICKEY, QTP, University of Florida — We work toward the development of orbital-free density functionals for the Kohn-Sham kinetic energy T_s of a quality suitable for the computation of quantum-mechanical forces in multi-scale molecular dynamics simulations. The functionals are based on constraints applicable to the Pauli potential $v_\theta = \delta T_\theta / \delta n$, where $T_s = T_w + T_\theta$ and T_w is the von Weizsäcker kinetic-energy functional. We review our progress to date, and exhibit functionals that do not generate spurious singularities and that produce chemical bonding in semi-quantitative agreement with Kohn-Sham computations and relevant experiments.

[1]Supported by U.S. NSF Grants PHY-0601758 and DMR-0325553

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Date submitted: 20 Nov 2008 Electronic form version 1.4