Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Benchmarking Density Functional Theory with Density Matrix Renormalization Group and Lessons For Higher Dimensions[1] THOMAS E. BAKER, Department of Physics and Astronomy, University of California, Irvine, California 92697 USA, LUCAS O. WAGNER, Department of Theoretical Chemistry and Amsterdam Center for Multiscale Modeling,FEW, Vrije Universiteit, De Boelelaan 1083, 1081HV Amsterdam, The Net, E. MILES STOUDENMIRE, Perimeter Institute for Theoretical Physics, Waterloo, Ontario, N2L 2Y5 Canada, STEVEN R. WHITE, Department of Physics and Astronomy, University of California, Irvine, California 92697 USA, KIERON BURKE, Department of Chemistry, University of California, Irvine, California 92697 USA — Kohn-Sham Density Functional Theory (DFT) is a mathematically exact method that requires approximation to the exchange correlation energy which may exclude features seen in experiment or provide inadequate estimates. Meanwhile, we may use Density Matrix Renormalization Group (DMRG), a numerical method which can accurately treat strongly correlated electrons in one dimension, to find exact DFT quantities such as the Kohn-Sham potential [1]. We use DMRG in one dimension as a benchmark to test new functionals. Further, recommendations for calculations in two and three dimensional systems are discussed as well as computational proof of principles [2]. [1] E.M. Stoudenmire, et. al., *Phys. Rev. Lett.* **109**, 056402 (2012) [2] Lucas O. Wagner, et. al., *Phys. Rev. Lett.* **111**, 093003 (2013)

[1]We graciously acknowledge the support of the Department of Energy (DE-SC0008696). L.O.W. also thanks the Korean Global Research Network Grant (No. NRF-2010-220-C00017).

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Date submitted: 14 Nov 2013 Electronic form version 1.4