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Electronic structure via potential functional approximations ATTILA CANGI, Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle (Saale), Germany, DONGHYUNG LEE, Department of Chemistry, Rice University, 6100 Main Street, Houston, TX 77005-1892, USA, PETER ELLIOTT, Department of Physics and Astronomy, Hunter College and the City University of New York, 695 Park Avenue, New York, New York 10065, USA, KIERON BURKE, Department of Chemistry, University of California, 1102 Natural Sciences 2, Irvine, California 92697-2025, USA, E.K.U. GROSS, Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle (Saale), Germany — The universal functional of Hohenberg and Kohn is given as a coupling-constant integral over the density as a functional of the potential [1]. Conditions are derived under which potential-functional approximations are variational. Construction via this method and imposition of these conditions are shown to greatly improve the accuracy of the non-interacting kinetic energy needed for orbital-free Kohn-Sham calculations. This result provides a direct route to a self-consistent, orbital-free theory for the electronic structure of matter within the Kohn-Sham framework. It solely requires an approximation to the non-interacting density as a functional of the potential, which, so far, has been derived for simple systems [2,3].

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