Abstract Submitted
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Exact Conditions in Finite-Temperature Density-Functional Theory[1] S. PITTALIS, Department of Physics and Astronomy, University of Missouri, Columbia, Missouri 65211, USA, C.R. PROETTO, Centro Atomico Bariloche and Instituto Balseiro, 8400 S. C. de Bariloche, Argentina, A. FLORIS, Department of Physics, King's College London, London, Strand WC2R 2LS, United Kingdom, A. SANNA, C. BERSIER, Max-Planck-Institut fuer Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany, K. BURKE, Department of Chemistry, University of California, Irvine, CA 92697, USA, E.K.U. GROSS, Max-Planck-Institut fuer Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany — Density-Functional Theory (DFT) for electrons at finite-temperature is increasingly important in condensed matter and chemistry. The exact conditions that have proven crucial in constraining and constructing accurate approximations for ground-state DFT are generalized to finite-temperature, including the adiabatic connection formula [1]. We discuss consequences for functional construction.

[1] S. Pittalis, C. R. Proetto, A. Floris, A. Sanna, C. Bersier, K. Burke, and E. K. U. Gross, Phys. Rev. Lett, 107, 163001 (2011)

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