

Abstract Submitted  
for the MAR11 Meeting of  
The American Physical Society

**Koopmans' condition for density-functional theory** ISMAILA DABO, CERMICS, University Paris-Est, ANDREA FERRETTI<sup>1</sup>, NICOLAS POILVERT, Department of Materials Science and Engineering, Massachusetts Institute of Technology, YANLI LI, Department of Physics, Xiamen University, NICOLA MARZARI<sup>2</sup>, Department of Materials Science and Engineering, Massachusetts Institute of Technology, MATTEO COCCIONI, Department of Chemical Engineering and Materials Science, University of Minnesota — In approximate Kohn-Sham density-functional theory, self-interaction manifests itself as the dependence of the energy of an orbital on its fractional occupation. Here, we first examine self-interaction in terms of the discrepancy between total and partial electron removal energies, and then highlight the importance of imposing the generalized Koopmans' condition to resolve this discrepancy. In the process, we derive a correction to approximate functionals that, in the frozen-orbital approximation, eliminates the unphysical occupation dependence of orbital energies up to the third order in the single-particle densities. This non-Koopmans correction brings physical meaning to single-particle energies; when applied to common local or semilocal density functionals it provides results that are in excellent agreement with experimental data while providing an explicit total energy functional that preserves or improves on the description of established structural properties.

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Date submitted: 02 Nov 2010

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