A DFT-based solution to the gap problem of antiferromagnetic transition metal oxides and parent compounds of high-$T_c$ superconductors

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Abstract

Presently used approximations to the exchange-correlation potential in Density Functional Theory (DFT) are known to fail in describing the properties of certain compounds of which we discuss here only two examples: CoO and stoichiometric La$_2$CuO$_4$. Both materials are insulating and antiferromagnetic. A DFT-calculation on CoO yields antiferromagnetic order, but Co-associated magnetic moments that are by $\sim 1\mu_B$ smaller than the experimental value, and one obtains the electronic structure of a metal. The latter applies also to La$_2$CuO$_4$, and - in contrast to the experiment - the calculation does not even yield non-zero moments associated with the Cu-atoms. We exploit the fact that approximate exchange-correlation potentials lead necessarily to spin-dependent densities that differ from the exact ones. We therefore derive modified Kohn-Sham (KS-)equations in which the effective potentials depend on the exact spin-densities rather than on the standard KS-densities. If the latter are modified by adding small (spin-up, spin-down) portions that individually integrate to zero within the lattice unit cell and do not change the total charge density, the inconsistencies with the experiment can be removed.

PACS: 31.10.+z 71.10.-w 71.15-m 71.15Mb 71.20-b 75.50E