Constrained RPA Study of Screened Electron Interactions in One-Dimensional Oxides

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DFT+*U* calculations and the constrained random phase approximation (cRPA) [1] have been used to study the Coulomb interaction screening in one-dimensional magnetic transition metal oxides XO_2 (X = Mn, Fe, Co, and Ni) adsorbed on the missing-row Ir(100)-1x3 surface.

The expected screening produced by the metallic substrate is combined with that by the O(*p*) ligands in a non-additive manner. This problem is tackled with the basis-set-independent method of Ref. [2] to isolate the correlated space from the rest of the Hilbert space in the cRPA calculations, together with the “shell folding” renormalization approximation [3].

Calculations on the free-standing chains allow us to understand the O(*p*) ligand contribution. In the case of NiO_2, two Hubbard *U* parameters are determined by cRPA that are associated to two possible Ni(*d*) electronic configurations (i.e., multiplets) of spin *S*=1/2. These values are *U*=2.4 and 6.4 eV. Interestingly, the low-*U* and high-*U* regimes can be identified with the Mott-Hubbard (*d*-*d* gap) and charge-transfer (*p*-*d* gap) regimes of the Zaanen-Sawatzky-Allen (ZSA) diagram [4], respectively. Upon adsorption on Ir, a low *U* value is found (*U*=1.7 eV), which is in part explained by the preference of the *p*-*d* gapped band structure.

The electronic structure of the MnO_2 chain is almost not altered by interaction with Ir. This situation helps to isolate the metal screening contribution, which is estimated with the aforementioned methods to be 0.9-1.4 eV.

References:

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