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Origin of band gaps in *3d* transition metal perovskite oxides

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With their broad range of properties, oxide perovskite of ABO3 general formula, where B is a 3d transition metal element, are materials of technological importance but also a platform for testing our solid state physics theories. Despite partly filled 3d states, most 3d transition metal oxide perovskites are insulating in both their high temperature spin-disordered paramagnetic state and their low temperature spin-ordered state. These insulating states are usually ascribed to strong dynamical correlation effects codified by the onsite repulsion U appearing the celebrated Hubbard model. It follows that theoretical technics modeling such effects are required to capture the physics of perovskites, thereby disqualifying density functional theory (DFT) that treat correlations only at the mean-field static level.

In this presentation, we show that if symmetry lowering events such as octahedra rotations and/or intrinsic electronic instabilities such as Jahn-Teller and disproportionation effects are properly included in the DFT simulations, the insulating or metallic character, the magnetic moments and the crystallographic structures are properly reproduced by DFT, both in the low and high temperature phases. We identify four mechanisms opening the band gap, none of them relying on strong dynamical correlation effects. Thus, the celebrated Hubbard model is likely not the universal explanation of the properties of perovskite oxides. Consequently, DFT is therefore qualified for studying doping, strain or interfacial effects in complex oxides.

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