"Orbital interactions and frustration in Jahn-Teller materials"

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Abstract

I show that the widely used model of exchange interactions in transition metal oxides is incomplete. It misses an important term, due to which the type of orbital ordering depends on the nature of the charge gap, i.e. an ordering in a charge transfer insulator may significantly differ from that in a Mott-Hubbard insulator. An inherent feature of the orbital exchange interactions is frustration. It results mainly from the strong anisotropy of the orbital exchange and occurs in materials with various crystal lattices, e.g. layered compounds with a triangular lattice (LiNiO\$_2\$) and cubic perovskites (KCuF\$_3\$). The structural and magnetic properties of Jahn-Teller materials essentially depend on mechanisms lifting this frustration.