Orbital fluctuation induced rich electronic properties in transition metal oxides

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Orbital fluctuation in the partially-filled t_{2g} manifold of orthovanadates $LaVO_3$ and YVO_3 at the room temperature acts as the trigger for the evolving nature of Jahn-Teller distortion in the orthorhombic and monoclinic phases. Equally important is the complex interplay of this JT distortion with the orthorhombic distortion whereby a variety of orbital ordering pattern is observed . This leads to the rich magnetic phase diagram in both the orthovanadates.[1] Hollandite $K_2Cr_8O_{16}$ shows a rare transition, namely from a ferromagnetic metal to a ferromagnetic insulator at 95 K. Electronic structure calculations within Local density approximation using the Nth-order MTO method[2] show that orbital fluctuation among the t_{2g} orbitals is pronounced in the ferromagnetic metal phase. Structural optimization using pseudopotentials with the Siesta package [3], including strong correlations, yields a structure with three different types of Jahn-Teller distortion in the Cr-O octahedra. Cr ions, driven by orbital fluctuation, now of three types with valencies only marginally deviating from +3.75 value. These Cr ions form four-chain columns surrounding each Cr1-Cr2-Cr1-Cr3 tetramer and each of these chains has alternating short and long Cr-Cr bonds. This dimerization, driven by orbital fluctuation, opens up a gap in the t_{2g} manifold. The role of the one-dimensional K ion network will be discussed vis-a-vis the role performed by the rare-earth ions in the orthovanadates.

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