

Reconciling magnetism with valence state in mixed-valent $\text{VO}_2\text{F}_2@\text{HV}_{22}\text{O}_{54}$ with localized and unlocalized electrons

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Polyoxovanadate molecular clusters due to large structural variety and many oxidation states of vanadium exhibit very rich magnetic behaviour and therefore find many technological applications. In this contribution two complementary theoretical approaches: DFT and effective Hamiltonian calculations are used to elucidate magnetism of mixed-valent $\text{VO}_2\text{F}_2@\text{HV}_{22}\text{O}_{54}$ with localized and unlocalized electrons. Extending the simplified modeling presented in [1] by taking into account kinetic energy of itinerant electrons and results of DFT we demonstrate that this compound differs from other members of $\text{X}@\text{HV}_{22}\text{O}_{54}$ family ($\text{X}=\text{ClO}_4$, SCN) not only by the presence of ferro- and antiferromagnetic interactions, but also by the valence state.

References:

[1] K. Yu. Monakhov, O. Linnenberg, P. Kozłowski, J. van Leusen, C. Besson, T. Secker, A. Ellern, X. López, J. M. Poble, P. Kögerler, *Chemistry – A European Journal* **21**, 2387 (2015)