LOCALIZED VS. ITINERANT ELECTRONS IN GaV₄O₈

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Summary: Mixed-valent transition-metal compounds display complex structural, electronic and magnetic properties, which often intricately coexist. Here, we report the new ternary oxide GaV₄O₈, a structural sibling of skyrmion-hosting lacunar spinels.

GaV₄O₈ crystallizes in a hexagonal structure, S.G. P63mc, with a = 5.667(1) Å and c = 9.356(1) Å cell parameters. Although the cooperative polar arrangement of GaO₄ Tetrahedra (Td) remains, it differs from the lacunar spinel in the X stacking sequence (ABC) being ABAC for the oxide.

GaV₄O₈ reveals the smallest vanadium trimer known to date (2.52 Å vs 3.14 Å for V-V distances) and an original spin-orbital-charge texture that forms upon the structural phase transition at Tₛ = 68 K followed by the magnetic transition at Tₙ = 35 K. The texture arises from the simultaneous presence of orbital molecules on the vanadium trimers and localized electrons on the remaining vanadium atoms. Such hybrid electrons create new opportunities for novel types of spin, charge, and orbital order in mixed-valent transition metal compounds.

Fig. 1 Comparison between GaV₄S₈ and GaV₄O₈ structures.