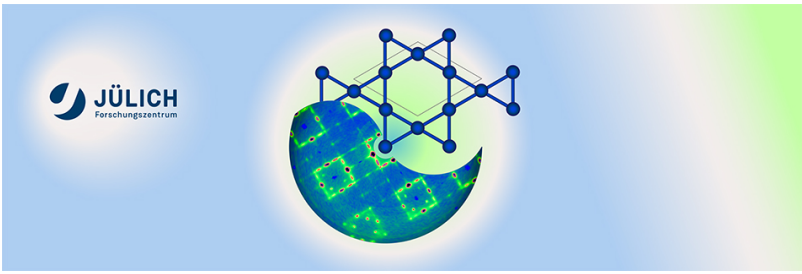

Beitrag ID: **89** Typ: **Talk**

Coupled charge, orbital, and spin degrees of freedom in geometrically frustrated YFe2O4

Mittwoch, 8. Oktober 2025 11:15 (15 Minuten)

Rhombohedral rare earth ferrites $R\mathrm{Fe_2O_4}$ have a strong tendency for coupled charge ($\mathrm{Fe}^{2+/3+}$) and spin order, despite the strong geometrical frustration of the interactions [1]. For R=Lu or Yb corresponding superstructure reflections or diffuse scattering appear at $(\frac{1}{3}\,\frac{1}{3}\,\ell)$. However, the size of Y^{3+} is considerably larger, with calculations [2] suggesting smaller in-plane propagation such as $(\frac{1}{4}\,\frac{1}{4})$.
Here, we focus on single-crystal x-ray diffraction performed on highly stoichiometric single crystals [3] of $\mathrm{YFe_2O_4}$. Magnetization vs T indicates two subsequent highly hysteretic magnetic transitions, separating a low-temperature (LT), an intermediate (IT), and a high-temperature (paramagnetic, HT) phase. XRD shows that these transitions are structural as well. In the HT phase, diffuse scattering at $(\frac{1}{3}\,\frac{1}{3}\,\ell)$ is similar to other rare earth ferrites. However, cooling into the magnetic phases, sharp superstructure reflections at different positions appear, with propagation $(\frac{2}{7}\,\frac{2}{7}\,\frac{3}{7})$ in IT and $(\frac{1}{4}\,\frac{1}{4}\,\frac{3}{4})$ in LT. We refined the superstructure in both phases and applied bond-valence-sum (BVS) analysis to probe the charge order [4].
In the LT phase, the structure is refined in P-1, with the inversion center between the two Fe layers. The BVS indicates a full charge order, with two of the Fe sites having valence close to 2+ and the other two close to 3+. Although of $(\frac{1}{4}\,\frac{1}{4})$-type, the arrangement of the valences differs from the prediction in [2]. Structural distortions also suggest (ferro) orbital order of the Fe^{2+} sites.
The IT phase is also refined in $P\bar{1}$. A clear splitting of one Y indicates the presence of disorder, which is likely connected to a fragile nature of this phase, which was not theoretically predicted. Of the 7 Fe sites, BVS shows 3 to have valences very close to 2+, indicating a strong localization of 3 electrons on these sites. However, the BVS of one of the sites is about 2.5, and for the remaining sites also further away from the ideal 3 (BVS~2.8). Thus the localization of electrons in the IT phase is incomplete, and it must be a dynamic situation with electron hopping occurring.

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Sitzung Einordnung: Frustrated spin systems

Track Klassifizierung: Frustrated spin systems