Orbital magnetism in van der Waals halide VI_3

Dávid Hovančík[1]
Jirí Pospíšil[1], Karel Carva[1], Vladimír Sechovský[1], Cinthia Piamonteze[2]
1 Charles University, Faculty of Mathematics and Physics, Department of Condensed Matter Physics, Ke Karlovu 5, 121 16 Prague 2, Czech Republic
2 Swiss Light Source, Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland
hovancik@mag.mff.cuni.cz

Van der Waals 3*d*-orbital ferromagnet with layered structure is a perfect research platform to achieve intrinsic 2D ferromagnetism and experimentally study the quantum nature of such a magnetic state. VI_3, a Mott insulator is an interesting example, with a complex magnetism and strong magnetic anisotropy distinguishing it from other 3*d*-based layered ferromagnets. So far, the existence of an unquenched orbital moment of V^{3+} ion that plays an essential role in the explanation of the magnetic ground state has been an open issue. We used the X-ray magnetic circular dichroism (XMCD) as a unique technique to probe the orbital moment component of the V^{3+} ion. Our results provide direct evidence for a significant orbital moment of the V^{3+} ion in VI_3 and point to the importance of spin-orbit coupling setting the electronic properties in the system. That sheds important light on the role of orbital magnetism in 2D systems. In addition, our ligand field multiplet simulations of XMCD spectra in synergy with DFT calculations propose the existence of two inequivalent V^{3+} sites with an opposite trigonal distortion and different orbital occupations.

Figures

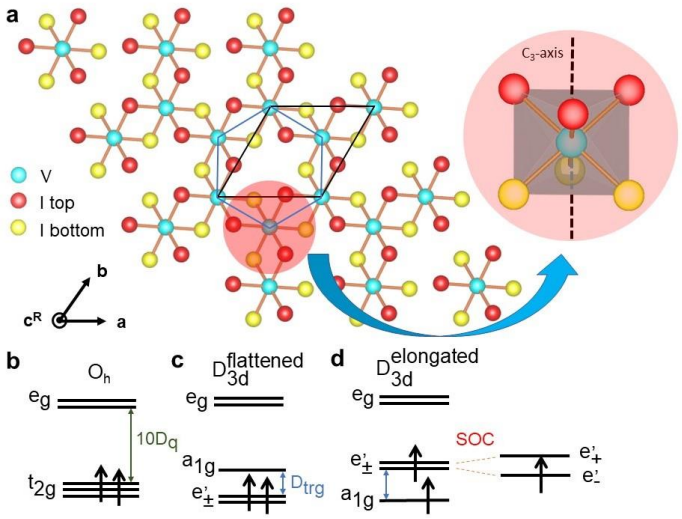

Figure 1: Crystal structure of VI_3 monolayer. The VI_6 cluster is emphasized (the three-fold axis C_3 is along the c^R-axis). b) c) and d) Crystal field splitting for O_h and D_{3d} (flattened/elongated octahedra) symmetry and corresponding electron occupation.