Optical d-d transitions in magnetic transition metal oxychlorides

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Two-dimensional (2D) magnetism, for many years were considered impossible to obtain due to strong thermal fluctuations [1]. That changed with experimental observation of magnetic order in 2D CrI_3 [2]. From that moment 2D magnets draw interest, especially in cases such as topology studies or detection and control of spin. Therefore exploring magnetic layered van der Waals (vdW) materials is crucial for understanding fundamental difference beetwen 2D and 3D ferromagnetism (FM) and antiferromagnetism (AFM) [3,4].

The transition metal oxychlorides (MOCl) are vdW semiconducting crystals exhibiting magnetic properties. In contrast to most of vdW magnets, which have a honeycomb structure with high lattice symmetry, MOCl have orthorombic structure characterized by higher anisotropy. It gives opportunity for more potential applications by addition of another degree of freedom in magnetism modulation [5].

In this work we present various spectroscopic measurements, such as transmission, reflection and photoacustic spectrocopy (PAS), of optical transitions in TiOCl, VOCl, CrOCl and FeOCl crystals. Experimental methods were supported by density functional theory (DFT) calculations. Optical absorption measurements along with PAS shows several absorption features in wide range from 1 to 4 eV. Comparison with DFT calculations allowed us to assigned them to specific band to band transitions.

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