Transition metal dihalides: from band structure to magnetic properties

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Abstract

Transition metal dihalides (TX_2) are quasi-2D magnets with weak inter-layer interaction. Their magnetic properties vary depending both on the filling of transition metal (T) $3d$ states and on the covalency of T d – X p bonds. Recently, monolayer-thick films of TX_2 dihalides were grown on various substrates allowing to study 2D magnetism. In this talk I shall show results of band structure calculations for bulk FeX_2 and NiX_2 dihalides. Calculations reproduce weak easy plane anisotropy in NiX_2 and the change of magnetic ground state within a layer from ferro- for $NiCl_2$ to helimagnetic for $NiBr_2$. The results of a fit of the total energies calculated for spin-spiral structures to the J_1–J_3, J_c Heisenberg model show that the change of the magnetic ground state is caused by the increased strength of J_3 in $NiBr_2$. Calculations for FeX_2 confirm, in agreement with experimental results, easy axis anisotropy. XMCD spectra calculated for both compounds are compared to experimental spectra for thin films. Calculated magnetic moments are compared to the experimental values extracted using XMCD sum rules.