Control of interactions in magnetic van der Waals materials via pressure

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Magnetic van der Waals materials offer a playground for external manipulation of its magnetic order. They are highly sensitive to applied pressure, which affects strongly the length of their weak interlayer bond and could lead to some other changes of the lattice. A highly interesting connection between the formation of helimagnetic order and breaking of both inversion and rotational symmetry of the lattice has been recently discovered in single-layer Ni dihalides [1]. Here we examine how the magnetic order in $NiBr_2$ is affected by pressure. We find a unique enhancement of the Néel temperature from 44 K at ambient pressure to 100 K at 3 GPa. Contrary to the NiI_2 case, the phase transition to helimagnetism rapidly shifts to lower temperatures with increasing pressure. We show that the interlayer exchange interaction plays here a key role in the selection of the most favorable magnetic order [2].

In CrI_3 bi- or tri-layers, pressure allows to even change the sign of interlayer interaction, switching between the ferromagnetic (FM) and layered antiferromagnetic (AFM) order [3]. Bulk CrI_3 with FM order exhibits initially an increase of Curie temperature with pressure, reaching a maximum near 3 GPa, which is followed by a decrease. The calculated Cr-I-Cr bond angle can explain the observed pressure dependence [4]. $CrBr_3$ behaves differently, it exhibits a steady decrease of Curie temperature with pressure, until the ferromagnetic order is completely destroyed. First principles calculations predict a weak decrease of the dominant exchange interaction in the range up to 8 GPa as long as the structure is unchanged, and also an increase of interlayer coupling with pressure. This leads to a pressure dependence of T_c that does not describe the experiment well. We propose a solution based on the presence of another phase with a different stacking and the preference for AFM order between layers, which is also indicated by x-ray scattering [5].

References:

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