Evolution of Structural, Magnetic and Electronic Properties with Pressure in TMPX₃ van-der-Waals Compounds

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We report discovery of new metallic and magnetic phases in the van-der-Waals antiferromagnets MPS3, where M = Transition Metal, form an ideal playground for tuning both low-dimensional magnetic and electronic properties[1-4]. These are layered honeycomb antiferromagnetic Mott insulators, long studied as near-ideal 2D magnetic systems with a rich variety of magnetic and electric properties across the family.

We will present magnetic, structural and electrical transport results and compare the behaviour of Fe-, V-, Mn- and NiPS3 as we tune them towards 3D structures – and Mott transitions from insulator to metal. I will show recent results on record high-pressure neutron scattering, which has unveiled an enigmatic form of short-range magnetic order in metallic FePS3.

We have mapped out the full phase diagram - a first in this crucial family of materials. We observe multiple transitions and new states, and an overall increase in dimensionality and associated changes in behaviour.

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Keywords: Magnetic Graphene, Mott Transitions, Insulator to Metal Transitions, Quantum Critical Systems