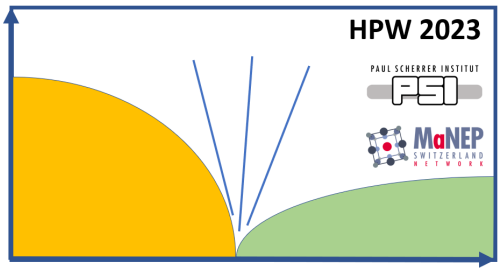


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# Pressure tuning and Evolution of Structural, Magnetic and Electronic Properties in TMPX3 van-der-Waals Compounds

*Wednesday, 22 November 2023 13:30 (15 minutes)*

Control of dimensionality in condensed matter continues to reveal novel quantum phenomena and effects. Transition metal phosphorous trichalcogenides *TM* P *X* 3 (*TM* = Mn, Fe, Ni, V, etc., *X* = S, Se) have proven to be ideal examples where structural, magnetic and electronic properties evolve into novel states when their dimensionality is tuned with pressure. At ambient pressure, they are two-dimensional van-der-Waals antiferromagnets with strongly correlated physics. Our recent experimental studies [1-4] have shown dimensionality crossover related pressure-induced insulator-to-metal transitions and novel magnetic phases in FePS3. To elucidate the relationship between structural transitions, magnetism and electronic properties, we also performed a random structure search using first-principles calculations at high pressures and DFT+U studies [5]. We experimentally explored the coexistence of the low- and intermediate-pressure phases, and we predict a novel high-pressure phase with distinctive dimensionality and possible options for interpreting the origins of metallicity.
We will also present our most recent single-crystal high-pressure synchrotron X-ray study on crystalline structures and the high-pressure neutron scattering study on magnetic structures of FePSe3, a similar compound to FePS3 with reported high-pressure induced superconductivity occurring at 2.5 K and 9.0 GPa [6]. The new work performed at the DIAMOND light source and Institut Laue Langevin finally provides clear crystallographic assignments related to phases which emerge with the application of pressure.

References:
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**Primary author:** DENG, Shiyu (University of Cambridge)

**Co-authors:** Dr R. S. HAINES, Charles (University of Cambridge; University of East Anglia); Dr J. COAK, Matthew (University of Cambridge; University of Birmingham); Dr HAMIDOV, Hayrullo (University of Cambridge;Navoi State University of Mining and Technologies); Dr DAISENBERGER, Dominik (Diamond Light Source); Dr WARREN, Mark (Diamond Light Source); Mr LIU, Cheng (University of Cambridge); Mr ZHANG, Xiaotian (University of Cambridge); Dr M. JARVIS, David (University of Cambridge; nstitut Laue-Langevin); Dr WILDES, Andrew (Institut Laue-Langevin); Prof. ARTACHO, Emilio (University of Cambridge; CIC Nanogune BRTA and DIPC; Ikerbasque, Basque Foundation for Science); Dr S SAXENA, Siddharth (University of Cambridge; British Management University)

**Presenter:** DENG, Shiyu (University of Cambridge)

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