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## Exploring d-d Transition Dynamics in FePS<sub>3</sub>: A Journey through Magneto-Optical and Photoelectron Spectroscopy Investigations



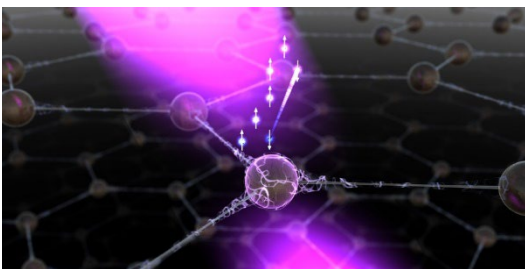
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Excitations between localized 3d states of transition metal ions within crystalline solids, commonly known as d-d transitions, play a pivotal role in diverse phenomena across solid-state physics, materials science, and chemistry. These transitions contribute significantly to the optical properties of transition metal oxides, catalytic activity on oxide surfaces, high-temperature superconductivity, and magnetic behaviors, facilitating spin-crossover transitions and linking optical excitation to quantized phenomena such as phonons and magnons. The discovery of unique effects in two-dimensional (2D) antiferromagnets, such as electron-phonon bound states, sub-terahertz (sub-THz) frequency magnon modes, and hybridized phonon-magnon modes, highlights the complex phenomenology driven by d-d transitions.

In this presentation, I will discuss our recent investigations into FePS<sub>3</sub>, selected for its promise as a scalable van der Waals antiferromagnetic semiconductor that retains magnetic order even at the 2D limit. We employed two complementary experimental approaches. Initially, pump-probe magneto-optical measurements were conducted to observe laser-driven lattice and spin dynamics. Pumping in resonance with a d-d transition within the Fe<sup>2+</sup> multiplet induced a coherent phonon mode oscillating at 3.2 THz. Remarkably, this mode is excitable in a low optical absorption regime, safeguarding even single antiferromagnetic layers from damage. The mode's amplitude diminishes with increasing temperature, disappearing at the Néel temperature as the system transitions to a paramagnetic phase, thereby illustrating its connection to long-range magnetic order. Furthermore, in an external magnetic field, this 3.2 THz phonon mode hybridizes with a magnon mode, enabling optical excitation of the resultant phonon-magnon hybrid mode [1].

Additionally, we utilized angle-resolved photoelectron spectroscopy (ARPES) to probe the electronic structure in its ground state [2] and employed time-resolved ARPES to capture the ultrafast dynamics of selected spin-allowed and spin-forbidden d-d transitions in FePS<sub>3</sub> [3]. The insights from magneto-optical experiments, juxtaposed with ARPES findings, shed light on the intricate quasiparticle dynamics underpinning d-d transitions in FePS<sub>3</sub>, offering a deeper understanding of their role in quantum material behaviors.



[1] F. Mertens, et al. *Advanced Materials* (2023). <https://doi.org/10.1002/adma.202208355>

[2] J.E. Nitschke, et al. *Materials Today Electronics* (2023). <https://doi.org/10.1016/j.mtelec.2023.100061>

[3] J.E. Nitschke, et al. *arXiv* (2024). [arXiv:2402.03018](https://arxiv.org/abs/2402.03018)