INSTITUT NEEL Grenoble

Proposition de stage Master 2 - Année universitaire 2024-2025

Theoretical investigation of 2D electron gases in novel layered materials

Reduced dimensionality in materials can lead to the emergence of novel properties. A particularly exciting example is the confinement of electrons to two dimensions, as 2D electron gases can exhibit intriguing phenomena such as superconductivity and charge-density waves. However, achieving such confinement typically requires sophisticated atomic-scale engineering. Recently, through a collaborative effort between theory and experiment, we discovered a new family of layered tungsten-phosphate compounds that display 2D electron gases stabilized by self-doping and antipolar distortions [1, 2].

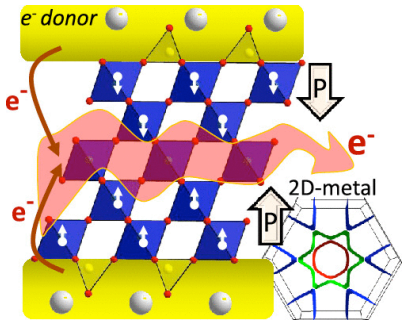

Figure 1: Stabilization of a 2DEG in novel layered tungsten-phosphates

In this project, we will utilize density functional theory to explore the relationship between structure and electronic properties in these compounds, with a specific focus on the dynamic stability and the electric and chemical control of the 2D electron gases, aiming to tune their properties.

[1] H. Nimoh, A. Cano et al, Angewandte Chemie International Edition 62 (25), e202302049 (2023)

[2] H. Nimoh, A.M. Arévalo-López, QN Meier, et al, Journal of the American Chemical Society 146 (34), 23955-23962 (2024)

Research topic and facilities available
The internship will be carried out at the Condensed Matter Theory (TMC) group at Institut NEEL. The available facilities include a HPC local cluster for the numerical calculations.

Possible collaboration and networking
The internship will be carried out in the framework of an ongoing national and international collaboration that includes theoreticians and experimentalists.

Possible extension as a PhD
Yes

Required skills
Theory. Solid state physics. Numerical calculations. Machine learning
Starting date 1/10/2024 (tentative)

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