# Unconventional 2D electron gases in novel quantum materials

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## General context

Reduced dimensionality in materials can lead to the emergence of novel properties. Of particular interest are two-dimensional electron gases (2DEGs) in transition-metal oxide materials, which can show strong electron correlations, and large spin-orbit coupling and generally show a complex interplay between spin, charge, and lattice degrees of freedom, and they can have been shown to host exotic electronic phases such as superconductivity, charge density waves and magnetism.

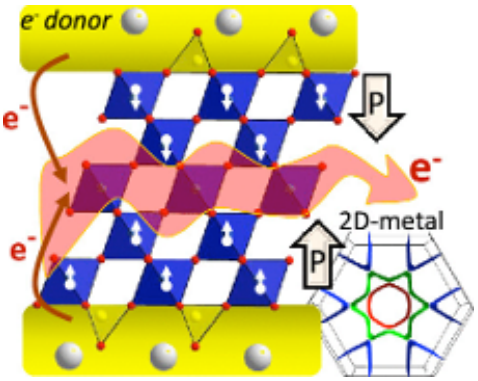


Figure 1: Schematics of the stabilization of a 2D Electron Gas in novel WO3-based materials.

In reality, achieving such strong 2D 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 novel mechanism combining self-doping and antipolar distortions [1, 2], a concept coined anti-polar 2D metallicity [2].

## Objectives of the PhD thesis

In this project, we will employ density functional theory (DFT)-based methods to characterize the structural and electronic properties of this novel material family and develop a general theoretical framework for the concept anti-polar 2D metallicity, with potential applicability to other layered systems. We will use our findings explore the tunability of the electron gases, focusing on their transport properties, spin-orbit effects, possible magnetic instabilities and superconducting phases, to assess their potential for novel electronic and quantum applications.

## Requirements

Strong background in condensed matter theory and numerical methods.
Experience with first-principles methods (DFT)
Programming skills (Python, C++, Fortran or others)

## References

[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, JACS 146 (34), 23955-23962 (2024)