First-principles characterization of superconductivity in 2D materials

Superconducting two-dimensional (2D) materials are attracting increasing interest, in view of fundamental changes in the superconducting properties due to quantum confinement, as well as for possible application as building blocks for new quantum technologies.

In this thesis, you will focus on MXenes, an emerging family of 2D materials, comprising transition metal carbides and nitrides. To gain insight in the microscopic origin of superconductivity in MXenes, you will perform first-principles calculations within the framework of density functional theory (DFT). This will enable you to fully characterize their electronic structure, phonon dispersion, and the electron-phonon interaction which mediates Cooper-pair formation. Next, you will use these results as input to perform advanced quantum-field calculations of the superconducting state, incorporating multiband effects and anisotropy of the pairing. You will also explore how the superconducting properties of MXenes can be tailored by surface decoration with dopants such as hydrogen and chlorine.