Title : Structural, electronic and magnetic instabilities in two-dimensional complex oxides		
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Research Area : Condensed Matter Physics and Materials Science		
Methods: Density functional theory based first principles calculations		

PhD track subject :

Nature seems to abhor high symmetry and large degeneracy. In condensed matter systems, this attitude is manifested as phase transitions when temperature or pressure is varied. Often, phase transitions are easily observed in thermodynamic experiments such as heat capacity and magnetization measurements. However, the order parameter of the broken-symmetry phase and the microscopic interaction causing the phase transition might be difficult to identify. Investigations of several such materials systems lie at the frontier of condensed matter physics.

This thesis will focus on the class of materials with layered structures that exhibit such subtle phase transitions. Examples include, but are not limited to, $NdNiO_2$, Na_xCoO_2, and $PdCrO_2$. The examples are chosen because they exhibit an enigmatic array of low temperature phases with unusual charge, spin and orbital orderings that are not fully understood. The objective of this thesis is to understand the structural, electronic and magnetic instabilities in such two-dimensional transition oxides that are challenging our current understanding of the condensed matter.

The student will learn to use density functional theory based first principles methods that take into account the specific chemical composition and crystal structure of the materials while studying their phase transitions. The instabilities causing the transitions will be identified by calculating microscopic quantities like Fermi surface, phonon dispersions and electron-phonon couplings. The role of these instabilities in breaking the crystal symmetries will be understood so that specific results can be generalized to similar materials systems.

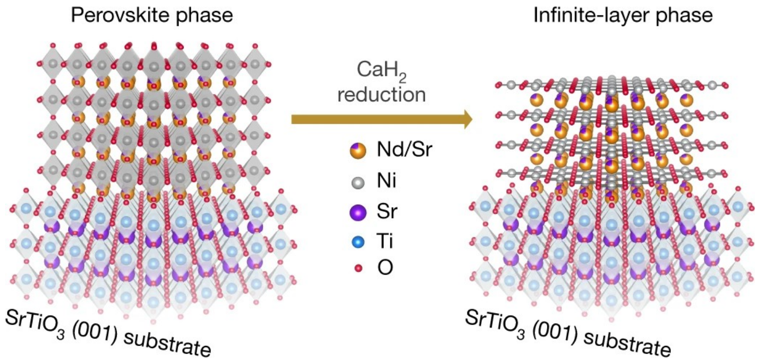

Figure 1: Thin-films of rare-earth nickelates become superconducting when the oxygen ions lying on the rare-earth layers are removed. The mechanism of superconductivity in this phase is not understood.

References:

[1] D. Li *et al.*, "Superconductivity in an infinite-layer nickelate", Nature 572, 624 (2019).
[2] P.J.W. Moll *et al.*, "Evidence for hydrodynamic electron flow in $PdCoO_2$", Science 351, 1061 (2016).