Symposium on Quantum Materials Synthesis, Porto, October 22 - 24, 2025

Surface effects in infinite-layer nickelate films

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Nickelates show intriguing similarities to cuprates, and have emerged as a compelling platform for studying high temperature superconductivity [1]. Infinite-layer rare-earth (R) nickelates, $RNiO_2$, consist of an alternating stacking of NiO_2 layers and rare-earth spacing layers along the crystallographic *z*-axis. While their bulk structure has been extensively studied computationally, the samples that exhibit superconductivity in experiments are thin nickelate films synthesized through a chemical reduction process. The topotactic reduction removes apical oxygen from perovskite $RNiO_3$, grown on substrates such as $SrTiO_3$ (001) [2].
Here, we explore emerging surface effects in $RNiO_2$ films by studying the formation and electronic structure of various surfaces within the framework of density functional theory (DFT) and dynamical mean-field theory (DMFT).
While perfect stoichiometry favors a NiO_2-terminated surface, the presence of excess apical oxygen in the surface region – possibly a remnant of the chemical reduction process – might stabilize an RO-terminated surface. Furthermore, the atomic structure at the surface is found to strongly influence the local electronic structure. These surface effects indicate the absence of an electron pocket around the Γ point – even for $NdNiO_2$ surfaces, in contrast to DFT and DMFT bulk calculations for $NdNiO_2$ [1].

We acknowledge support through a joint German and Austrian Science Funds (DFG and FWF) project; FWF Grant-DOI:10.55776/I5398.

References:

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