Site-selective polar compensation of Mott electrons in a double perovskite heterointerface

Srimanta Middey
Department of Physics, Indian Institute of Science, Bengaluru 560012, India

Double perovskite oxides (DPOs) with two transition metal ions ($A_2BB'O_6$) offer a fascinating platform for exploring exotic physics and practical applications. Studying these DPOs as ultrathin epitaxial thin films on single crystalline substrates can add another dimension to engineering electronic, magnetic, and topological phenomena. Understanding the consequence of polarity mismatch between the substrate and the DPO would be the first step towards this broad goal. We investigate this by studying the interface between a prototypical insulating DPO Nd_2NiMnO_6 and a wide-band gap insulator $SrTiO_3$. The interface is found to be insulating in nature. By combining several experimental techniques and density functional theory, we establish a site-selective charge compensation process that occurs explicitly at the Mn site of the film, leaving the Ni sites inert. We further demonstrate that such surprising selectivity, which cannot be explained by existing mechanisms of polarity compensation, is directly associated with their electronic correlation energy scales. This study establishes the crucial role of Mott physics in polar compensation process and paves the way for designer doping strategies in complex oxides.

1. Bhattacharya,..Middey et al., Site-selective polar compensation of Mott electrons in a double perovskite heterointerface, *Phys. Rev. Lett., in press (2025).*
2. Bhattacharya,....Middey et al., Interfacial reconstruction effects in insulating double perovskite $Nd_2NiMnO_6/SrTiO_3$ and $Nd_2NiMnO_6/NdGaO_3$ thin films, *under review (2025).*