MIP: PARADIM at Cornell University, DMR-2039380 In-House Research Project - 2024

REU students have a multitude of backgrounds but share a common thirst: to do cutting-edge research. As part of its 10-week immersion in hands-on research, PARADIM encourages its REU students to dive in and learn new techniques at the same time they experience the power of team-based research. Such a team has been studying low-dimensional metallic delafossites, with the general formula ABO_2 , with the goal of producing electronic and magnetic characteristics that are not accessible in single crystals of these materials. These layered structures consist of alternating monolayers of Pt or Pd alternating with monolayers of CoO₂ or CrO₂ and have conductivities that are the highest of any oxide—surpassing those of Pt and Pd metals even.

Together with its REU students, the PARADIM In-House Team successfully synthesized high-quality $PtCoO_2$, $PdCoO_2$, and $PdCrO_2$ films by MBE, followed by a comprehensive investigation of their surface reconstructions using a combination of ARPES, LEED, and RHEED, plus assessment of the structural quality (by AFM, XRD, and TEM) and their electronic conductivity as a function of thickness. New surface reconstructions were seen. First-principles calculations from PARADIM's theory user facility shed light on the relative instability of surfaces terminated with A (A = Pt, Pd) atoms compared to those terminated with BO_2 (B = Co, Cr), as evidenced by their higher formation energies.

This work sets the stage for further exploration of highly twodimensional studies in this intriguing class of quantum materials.

Q. Song, et al., <u>APL Mater. 12</u>, 081117 (2024).

ORATE FOR MATHEMATICAL AND PHYSICAL SCIENCES

Materials Discovery is a Team Sport for All Ages



Kyle M. Shen, Darrell G. Schlom, and Craig J. Fennie (PARADIM)

Figure: The surface of $PtCoO_2$ studied by (left) two types of electron diffraction (LEED and RHEED) showing a change in atomic structure on the surface of the film compared to the underlying atomic layers. (center) Angle-resolved photoemission spectroscopy is used to reveal

how the electrons are moving in the $PtCoO_2$ film, including the effect of the altered surface structure. (right) Photographs of the **three PARADIM REUs** who are among the co-authors.



Where Materials Begin and Society Benefits



Sonia Hasko