Coexistence of Dirac and flat bands in 2D material beyond geometrical frustrated lattice

Asish K. Kundu[1], Christie S. Koay[2], Daniel G. Chica[2], A. Devarakonda[2], Anil Rajapitamahuni[1], Raquel Queiroz[2], Xavier Roy[2], Abhay N. Pasupathy[2], and E. Vescovo[1]

[1]*Brookhaven National Laboratory, Upton, NY, USA*
[2]*Columbia university, New York, NY, USA*

Two-dimensional (2D) Dirac materials featuring flat bands have emerged as a pivotal focus in condensed matter physics due to their rich physical phenomena, including superconductivity and ferromagnetism, and their potential for integration into electronic devices. Flat bands, typically associated with strong electron correlations, are predominantly observed in heavy fermion systems with localized *f*-orbitals. While geometrically frustrated lattices have been proposed as a pathway to extend bulk flat bands beyond *f*-orbital systems, to date, such bands have only been identified in solid-state materials with kagome and related pyrochlore lattice structures. Here, I will present our recent study [1] unveiling the coexistence of Dirac and flat bands within the geometrically unfrustrated primitive square lattice compound Pd_5AlI_2, investigated through angle-resolved photoemission spectroscopy (ARPES) and model calculations. Theoretical calculations and polarization-dependent ARPES measurements reveal that specific atomic orbital decorations on a primitive square lattice induce frustrated electron hopping, forming a flat band. Further, photon-energy dependence of electronic structure measurements shows the quasi-2D electronic nature of this material. Owing to the van der Waals (vdW) nature, this material can be exfoliated to the monolayer limit, paving the way for exploring orbital physics in true 2D limit.

Keywords: 2D vdW metal, electronic structure, ARPES, flat band, Dirac material, density functional theory, materials discovery.

Acknowledgement: ARPES measurements used resources at the 21-ID (ESM) beamline of the National Synchrotron Light Source II, a U.S. Department of Energy (DOE) Office of Science User Facility operated for the DOE Office of Science by Brookhaven National Laboratory under Contract No. DE-SC0012704. Research on novel hopping models was conducted as part of the Programmable Quantum Materials, an Energy Frontier Research Center, funded by the US Department of Energy (DOE), Office of Science, Basic Energy Sciences, under award DE-SC0019443 (X.R., A.N.P., R.Q.). The synthesis and structural characterization of the 2D metal was supported by the NSF MRSEC program through the Center for Precision-Assembled Quantum Materials at Columbia University, award number DMR-2011738 (X.R., A.N.P). A.D. acknowledges support from the Simons Foundation Society of Fellows (grant No. 855186).

[1]A. Devarakonda, Christie S. Koay, Daniel G. Chica, M. Thinel, Asish K. Kundu et al., "*Frustrated hopping from orbital decoration of a primitive two-dimensional lattice*", arXiv preprint, arXiv:2408.01512 (2024).