Magnetic Interfaces and Nanostructures
Room Ballroom A - Session MI-ThP

Magnetic Interfaces and Nanostructures Poster Session

MI-ThP-1 Wilson Loop as a Tool to Investigate Chirality-Induced Spin Selectivity: Role of Vibrations and Multiple Channels, ***Leonardo Celada****, D. K. Andrea Phan Huu, Alessandro Chiesa, Paolo Santini, Luca Griguolo, Stefano Carretta,* Università degli studi di Parma, Italy

Chirality-induced spin selectivity (CISS) has been observed in a wide range of chiral molecular systems, yet the minimal microscopic ingredients required for spin polarization remain debated [1]. Here we introduce the Wilson loop as a general theoretical criterion to identify when spin polarization can emerge in model Hamiltonians relevant to CISS.

Using open tight-binding models with spin-orbit coupling, we show that the Wilson loop provides a gauge-invariant characterization of spin-dependent interference and recovers the known absence of CISS in single-channel purely electronic models, where a local spin gauge transformation removes all spin dependence. By contrast, non-trivial Wilson loops arise in systems with multiple transport channels, providing a direct symmetry-based criterion for finite spin polarization, consistent with previous theoretical studies of CISS mechanisms [2].

We then extend this framework to electron-vibration models and show that vibronic pathways can generate non-trivial Wilson loops even in nominally single-channel systems. In particular, Peierls-type coupling creates spin-dependent interference in vibronic space and enables CISS, whereas Holstein coupling preserves a trivial Wilson loop and cannot induce spin polarization. This establishes a distinction between vibrational mechanisms proposed in the literature [3].

Beyond reproducing known results, the Wilson-loop formulation provides a unifying path-based picture connecting gauge structure, interference, and spin selectivity across electronic and vibronic mechanisms. The framework can be generalized to arbitrary molecular architectures and offers a tool to identify necessary conditions for CISS in transport and electron-transfer settings, including systems where spin selectivity has recently been observed experimentally [4].

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References

[1] Naaman, R. Nat. Rev. Chem. 2019, 3, 250.
[2] Chiesa, A. Nano Lett. 2024, 24, 12133–12139.
[3] Fransson, J. *Phys. Rev. B* **2020**, *102*, 235416.
[4] Eckvahl, H. J. Science 2023, 382, 197–202.

MI-ThP-4 Early-Stage Experimental Training in Magnetism: A Hands-On Freshman Research Course as a Gateway to Advanced Magnetic Materials, ***Mikel Holcomb****,* West Virginia University*; Femi Akinrinola,* West Virginia University, USA*; Robbyn Trappen, Seth Woodwyk, Ivan Gray, Tap Raj Bhandari, Jeremy Fanelli, Dorian Davis, Nethmi Kankanamge, John Stewart,* West Virginia University

The development of advanced magnetic materials and low-dimensional magnetic systems relies critically on a skilled experimental workforce capable of integrating measurement and data interpretation at early stages of training. I describe a hands-on freshman-level research course designed to introduce students to experimental magnetism through direct engagement with measurement techniques and a variety of magnetic systems. In this course, students perform studies on magnetic materials, with an emphasis on data acquisition and physical interpretation. Projects are structured to connect fundamental concepts—such as magnetic anisotropy, hysteresis and types of magnetism—to experimental observables, providing an entry point into phenomena central to modern magnetism research. Students develop experimental intuition through open-ended investigations that reflect the uncertainty and exploratory nature of contemporary research, with each project structured as a potentially extensible research direction. I will discuss course design, representative experiments, and evidence for improved student readiness for research in physics and materials science. This model suggests a pathway for broadening participation and accelerating training in areas aligned with emerging challenges in magnetic interfaces and nanostructures. This work is supported by NSF DUE 2417349.

MI-ThP-5 First- Principles Study of Strain- Controlled Magnetism in MnBi2Se4 Heterostructure, ***Narendra Phulara,*** University of Kansas

Abstract : We present a first-principles study of the magnetic ground state of the magnetic quantum material $MnBi_2Se_4$ supported on a ferroelectric substrate. Using density functional theory, we will first compare ferromagnetic and antiferromagnetic configurations of freestanding $MnBi_2Se_4$. We will then obtain a fully relaxed slab structure of the ferroelectric substrate, construct the $MnBi_2Se_4$/substrate heterostructure, and determine its equilibrium geometry and magnetic ground state. Finally, shear strain will be applied to the relaxed heterostructure to examine how structural deformation modifies the relative stability of the ferromagnetic and antiferromagnetic states. This systematic study will establish whether shear strain provides an effective route for controlling the magnetic ground state of $MnBi_2Se_4$ in ferroelectric-based heterostructures for potential spintronic applications.

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