Harnessing frustrated magnetism in honeycomb cobaltates

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The realization of Kitaev magnetism and quantum spin liquid phases in solid-state compounds has remained elusive due to the presence of various magnetic energy scales that reduce symmetries and stabilize long-range orders. Recently, layered honeycomb cobaltates have gathered significant attention following theoretical predictions of potential Kitaev exchange interactions from Co d^7 high-spin states. While early suggestions of Kitaev interactions in compounds like BaCo2(AsO4)2 have been challenged by first-principles electronic structure calculations, interest in honeycomb cobaltates persists due to experimental reports of field-induced paramagnetic phases, which are speculated to be potential spin liquid states. In this study, we present our recent investigations into two distinct types of layered honeycomb cobaltates, BaCo2(PnO4)2 (Pn = P, As, Sb)[1,2] and Cu3Co2SbO6[3]. Our results, based on dynamical mean-field theory calculations, suggest the presence of spin-orbit-entangled J_eff=1/2 moments. Further we propose viable strategies, employing chemical substitutions and epitaxial strains, for tuning exchange interactions to enhance magnetic frustration in these systems.

[1] S. Samanta et al., Phys. Rev. B 106, 195136 (2022).
[2] S. Samanta, F. Cossu, H.-S. Kim, arXiv:2406.18003 (2024).
[3] G.-H. Kim et al., Sci. Adv. 10, eadn8694 (2024).