"Can we realize Kitaev quantum spin liquids in Jeff = 1/2 cobaltates ?"

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The quest for Kitaev quantum spin liquids has led to great interest in honeycomb quantum magnets with strong spin-orbit coupling. It has been recently proposed that even Mott insulators with 3d transition-metal ions, having nominally weak spin-orbit coupling, can realize such exotic physics. Motivated by this, we study the rhombohedral honeycomb cobaltates $CoTiO_3$, $BaCo_2(PO4)_2$, and $BaCo_2(AsO_4)_2$, using *ab initio* density-functional theory, which takes into account realistic crystal-field distortions and chemical information, in conjunction with exact diagonalization numerics. We find are these materials are in fact described by a pseudospin-1/2 easy-plane spin Hamiltonian with nearest neighbor ferromagnetic (FM) exchange J1 being frustrated by antiferromagnetic third-neighbor exchange J3 and weaker compass anisotropies, in contrast to initially proposed Kitaev quantum magnets.[1] Using exact diagonalization and density-matrix renormalization group (DMRG) calculations, we show that this model exhibits FM order at small J3/J1 and zig-zag (ZZ) order at large J3/J1, separated by an intermediate phase, which we label as *sl*. This *sl* phase is shown to exhibit spin-liquid-like correlations in DMRG.[2]

References:

[1] Shreya Das, Sreekar Voleti, Tanusri Saha-Dasgupta, Arun Paramekanti, Phys. Rev. B **104**, 134425 (2021).

[2] Anjishnu Bose, Manodip Routh, Sreekar Voleti, Sudip Kumar Saha, Manoranjan Kumar, Tanusri Saha-Dasgupta, Arun Paramekanti, Phys Rev B (in press)