Abstract Submitted
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Importance of anisotropy in the spin-liquid candidate $Me_3EtSb[Pd(dmit)_2]_2$[1] LUCA F. TOCCHIO, ANTHONY JACKO, HARALD O. JESCHKE, ROSER VALENTI, University of Frankfurt — Organic charge transfer salts based on the molecule $Pd(dmit)_2$ display strong electronic correlations and geometrical frustration, leading to spin liquid, valence bond solid, and superconducting states, amongst other interesting phases. The low energy electronic degrees of freedom of these materials are often described by a single band model; a triangular lattice with a molecular orbital representing a $Pd(dmit)_2$ dimer on each site. We use *ab initio* electronic structure calculations to construct and parametrize low energy effective model Hamiltonians for a class of Me_{4-n} $Et_nX[Pd(dmit)_2]_2$ (X=As, P, N, Sb) salts and investigate how best to model these systems by using variational Monte Carlo (VMC) simulations. Our findings suggest that the prevailing model of these systems as a $t-t'$ triangular lattice is incomplete, and that a fully anisotropic triangular lattice description produces importantly different results, including a significant lowering of the critical U of the spin-liquid phase.[1,2] [1] A.C. Jacko, L. F. Tocchio, H. O. Jeschke, R. Valenti, Phys. Rev. B 88, 155139 (2013). [2] L. Tocchio, H. Feldner, F. Becca, R. Valenti, C. Gros Phys. Rev. B 87, 035143 (2013).

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