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Microscopic models of Pd(dmit)$_2$-based organic charge transfer salts ANTHONY JACKO, HARALD O. JESCHKE, ROSER VALENTI, Institut für Theoretische Physik, Goethe-Unversität Frankfurt, Max-von-Laue-Str. 1, 60438 Frankfurt, Germany — 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=N, As, Sb) salts and investigate how well these systems are described by an anisotropic triangular lattice.

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