

Abstract Submitted
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Ground-state properties of $\text{EtMe}_3\text{Sb}[\text{Pd}(\text{dmit})_2]_2$ by many-variable variational Monte Carlo method SATOSHI MORITA, RYUI KANEKO, MASATOSHI IMADA, Department of Applied Physics, University of Tokyo — The organic Mott insulator $\text{EtMe}_3\text{Sb}[\text{Pd}(\text{dmit})_2]_2$ is a strongly correlated electron system on a nearly-regular triangular lattice and regarded as a spin liquid material. We investigate its effective low-energy model derived from first principles calculations and band+dimensional downfolding. The *ab initio* effective Hamiltonian is given in the form of the two-dimensional single-band extended Hubbard model on an anisotropic triangular lattice with short-ranged Coulomb and exchange interactions. Its ground state is calculated by the many-variable variational Monte Carlo method with quantum-number projection and multi-variable optimization. We draw the ground-state phase diagram as a function of scaling parameters for the interactions and the geometrical frustration by extending the *ab initio* model. We discuss Mott transitions and magnetic properties.

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