Geometrical frustration effects on the Mott transition in layered charge transfer organic compounds

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The effects of geometrical frustration in quasi-two-dimensional k-(BEDT-TTF)$_2$X crystals is investigated.
The minimal strongly correlated model to understand their properties, the Hubbard model on an anisotropic triangular lattice, is analyzed within the cellular dynamical mean-field theory (CDMFT) with finite temperature Lanczos diagonalization [1] as the impurity solver. We obtain the low temperature-pressure (T-P) phase diagram for different degree of geometrical frustration of the lattice. Coexistence regions of metallic and insulating phases around the Mott transition and absolute values of critical temperatures at the Mott transition are in good agreement with experimental findings [2]. The T-P phase diagram develops 'reentrant' behavior as the geometrical frustration of the lattice is released resulting from the enhancement of short range magnetic correlations. We discuss the implications of our results to k-(BEDT-TTF)$_2$X crystals.

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