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Ferroelectricity and magnetism in the organic charge transfer salts κ-$(ET)_2X$

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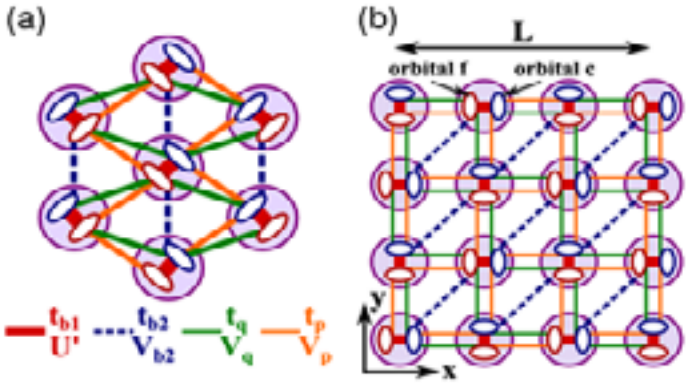
The molecular conductors κ-$(ET)_2X$, where ET denotes an organic molecule and X is an anion, exhibit electronic ferroelectricity, where charge order breaks inversion symmetry, accompanied by the onset of magnetic order. These materials can be modeled by a 3/4 filled extended Hubbard model on a two-orbital anisotropic triangular lattice (see figure), where the molecular degrees of freedom are explicitly taken into account. The model is theoretically investigated by the variational Monte Carlo method. By studying the effect of the competing inter-site Coulomb interactions, we determine charge order patterns and how these charge orders generate emergent magnetic order. In particular, we find three charge ordered phases, namely, a nonpolar insulating one, a polar insulating one, leading to ferroelectricity, and a charge-ordered metallic phase with a 3-fold geometry. The charge ordered phases are accompanied by the presence of magnetic order that is more enhanced within the polar phase.



Biography

Luca F Tocchio is a Researcher at the Institute for Condensed Matter Physics and Complex Systems of Politecnico di Torino. He has worked as a Post-doctoral fellow at the University of Frankfurt and at the International School for Advanced Studies (SISSA) in Trieste, where he also did his PhD. He works on numerical Monte Carlo simulations of models for strongly correlated electron systems, aiming to study topics like high-temperature superconductivity, spin-liquid phases, interplay between charge and magnetic degrees of freedom. He is also interested in methodological improvements of variational wave functions to better describe correlated electron systems.

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