Frustration in the charge transfer salts

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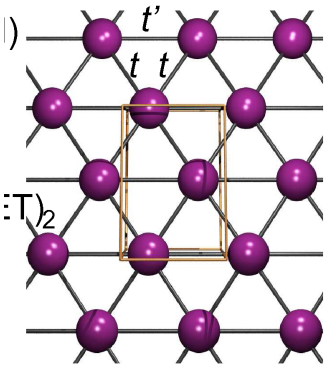
Intense experimental and theoretical studies have demonstrated that the anisotropic triangular as realized in the Kappa -(BEDT-TTF)2X family of organic charge transfer (CT) salts yields a complex phase diagram with magnetic, superconducting, Mott insulating and even spin liquid phases. With extensive density functional theory (DFT) calculations we refresh the link between many-body theory and experiment by determining hopping parameters of the underlying Hubbard model [1]. This leads us to revise the widely used semi-empirical parameters in the direction of less frustrated, more anisotropic triangular lattices. The implications of these results on the systems' description will be discussed and comparison to other Mott-Hubbard insulators will be shown [2].



Lattice of ET dimers in the Kappa -(BEDT-TTF)2X compounds

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[1] H. C. Kandpal, I. Opahle, Y.-Z. Zhang, H. O. Jeschke, R. Valenti, arXiv:0904.0302
[2] Y.-Z. Zhang, H. O. Jeschke, R. Valenti Phys. Rev. Lett. 101, 136406 (2008).