

Density Functional Parameterisation of the Hubbard Model as an Effective Low Energy Hamiltonian for Organic Charge Transfer Salts

Edan Scriven¹ and Ben Powell¹

¹Centre for Organic Photonics and Electronics, School of Mathematics and Physics, University of Queensland, Brisbane, 4072 Australia

Email: edan@physics.uq.edu.au

Organic charge transfer salts of the form (BEDT-TTF)₂X where X is a monovalent anion exhibit unusual physical phenomena, including a metal-insulator phase transition, spin liquid and unconventional superconductivity[1].

Density-functional theory (DFT) band structures of these materials fail to capture the physics of strong electron correlations. It is believed the Hubbard model captures the physics of the BEDT-TTF salts[1]. Therefore we focus on parameterising the Hubbard model.

We calculate the Hubbard U and site energy for electrons on a variety of BEDT-TTF monomers *in vacuo*[2]. We also calculate the intradimer Hubbard U for ET dimers in the β - and κ - polymorphs. DFT energies of BEDT-TTF monomers and dimers in various charge states were used to parameterise the Hubbard model. We discuss the significance of these calculations to understanding the physics of these materials.

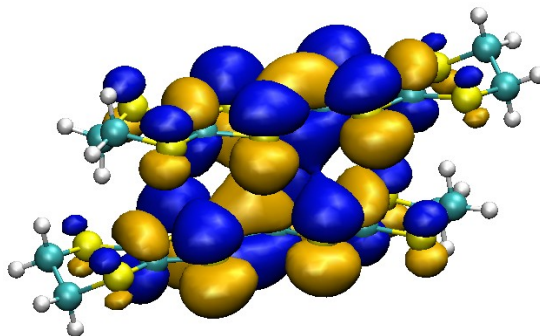


Figure 1: Highest-occupied molecular orbital of a BEDT-TTF dimer in the spin liquid material κ -(BEDT-TTF)₂Cu₂(CN)₃ in the charge neutral state.

[1] Powell, B.J., McKenzie, R.H., J. Phys. Cond. Mat. **18** (2006) R827.

[2] Scriven, E., Powell, B.J., J. Chem. Phys. **130** (2009) 104508.