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Realistic modeling of organic crystals

Organic crystals show a wide variety of unusual effects. Even though they do not contain any metal atoms they can be highly conducting, even superconducting, they have interesting magnetic phases, or show effects of low dimensionality. This rich physics is a result of electron correlations: The molecular orbitals in an organic crystal overlap only weakly, giving rise to quite narrow bands. Therefore the repulsion between electrons becomes so important that it cannot be described using mean-field approaches. The resulting many-body physics is exiting, but hard to treat theoretically. In practice we have to resort to model Hamiltonians, generalized Hubbard models, that consider only the conduction electrons.

For the example of \theta-(BEDT-TTF)2I3, we show how to systematically construct such a realistic Hubbard model. Based on density functional calculations, we discuss how to model the experimental crystal structure, and to determine hopping matrix elements. Using a classical screening approach we show how the screened Coulomb interaction can be calculated. We finally discuss how sensitive the model parameters are to structural changes.