

Screening of Coulomb repulsion energies in organic molecular compounds

Laura Cano-Cortés¹, Andreas Dolfen², Jaime Merino¹, and Erik Koch²

¹*Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, Spain*

²*Institut für Festkörperforschung, Forschungszentrum, Jülich, Germany*

Email: laura.canocortes@uam.es

Low dimensional organic molecular compounds based on the BEDT-TTF, TTF and TCNQ molecules are narrow band systems in which the Coulomb repulsion is comparable to the bandwidth. Accurate estimates of Coulomb parameters inside these organic crystals for Hubbard Hamiltonians are needed in order to have a realistic description of their electronic properties. The main screening mechanism in such organic compounds which is not included in the Hubbard model is the polarization of the surrounding molecules. An accurate estimate of the screening energy due to polarization can be achieved by realizing that the molecules preserve their identity inside the crystal and that their mutual interaction can be described through classical electrostatics [1]. Based on these assumptions, we present a general method for determining Coulomb parameters for organic molecular crystals and other molecular assemblies. Due to the slow convergence of the Coulomb interaction, we evaluate the dipole interaction energy of the infinite crystal efficiently through Ewald sums [1] which are then used to explore the screening properties and dipole arrangements in one-dimensional chains and simple cubic three-dimensional lattices. The method is applied to TTF-TCNQ salts finding that they are close to a ferroelectric instability which makes the point dipole description a poor approximation. However, using distributed dipoles over the TTF-TCNQ molecules is found to improve the description of the molecule [1] and accurate screened Coulomb parameters [2] can then be obtained.

*This work was supported by MICINN (project: CTQ2008-06720-C02-02).

[1] P. B. Allen, J. Chem. Phys. 120, 2951 (2004).

[2] L. Cano-Cortés, A. Dolfen, J. Merino, J. Behler, B. Delley, K. Reuter and E. Koch, Eur. Phys. J. B 65, 173 (2007).