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Realistic Parameters for the Description of Organic Metals ANDREAS DOLFEN, German Research School for Simulation Sciences, Germany, ERIK KOCH, Institut für Festkörperforschung, Forschungszentrum Jülich, Germany, VOLKER BLUM, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany, LAURA CANO-CORTÉS, JAIME MERINO, Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, Spain — In molecular crystals correlation effects are often significant. For a non-perturbative description of the full Coulomb interaction we have therefore to resort to a model description in terms of generalized Hubbard models. The derivation of parameters for such models is crucial for realistic simulations. While hopping parameters are easily derived from density-functional theory (DFT) the Coulomb parameters pose a significant problem due to screening processes. We decompose their contributions into intra- and inter-molecular parts. The intra-molecularly screened Coulomb parameters are treated within DFT whereas the inter-molecular corrections are evaluated using classical electrostatics with DFT-derived polarizabilities and the distributed-dipole approach in combination with a Ewald summation. Even for simple lattices of polarizable point dipoles we find intriguing screening phenomena. As realistic applications we discuss the one- and two-dimensional organic metals TTF-TCNQ and Θ-$(BEDT\text{-}TTF)_2I_3$.

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