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LDA+DMFT investigation of the organic charge transfer salt κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Cl JOHANNES FERBER, KATERYNA FOYEVTSOVA, HARALD O. JESCHKE, ROSER VALENTI, Institut für Theoretische Physik, Goethe-Unversität Frankfurt, Max-von-Laue-Str. 1, 60438 Frankfurt, Germany — We combine density functional theory with dynamical mean field theory for the study of organic molecular crystals using a new scheme to construct molecular Wannier functions. We calculate spectral and optical properties for the strongly correlated material κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Cl. The new method allows us to analyze the contributions of intradimer and interdimer contributions to the optical conductivity on the same footing. We find in agreement with experiment that strong correlations lead to a Hubbard peak in the optical conductivity.

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