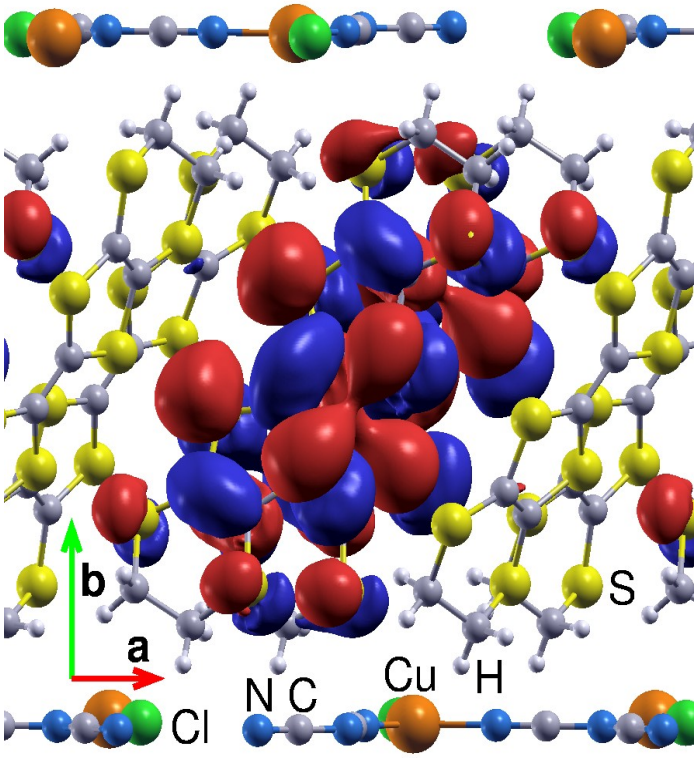
Realistic many-body calculations with spatial correlations and for systems with molecular orbitals

Harald O. Jeschke*, J. Ferber, K. Foyevtsova, Roser Valentí
Institut für Theoretische Physik, Goethe-Universität Frankfurt, Max-von-Laue-Str. 1, 60438 Frankfurt, Germany
*jeschke@itp.uni-frankfurt.de

While the combination of the local density approximation (LDA) with dynamical mean field theory (DMFT) opened the door to a realistic description of correlated compounds, a better description of the *k* dependence is clearly desirable. We present a combination of local density approximation (LDA) with the dynamical cluster approximation (LDA+DCA) in the framework of the full-potential linear augmented plane-wave method, and compare our LDA+DCA results for $SrVO_3$ to LDA with the dynamical mean field theory (LDA+DMFT) calculations as well as experimental observations on $SrVO_3$ [1]. We find a qualitative agreement of the momentum resolved spectral function with angle-resolved photoemission spectra (ARPES) and former LDA+DMFT results. We explain how the different properties of the **K** sectors already at the LDA level lead to differences between LDA+DMFT and LDA+DCA due to the sector dependent self energies present in DCA.

For the study of organic molecular crystals, we combine density functional theory with dynamical mean field theory using a new scheme to construct molecular Wannier functions (see illustration). 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 [2].



[1] H. Lee, K. Foyevtsova, J. Ferber, M. Aichhorn, H. O. Jeschke, R. Valentí, *Dynamical cluster approximation within an augmented plane-wave framework: Spectral properties of $SrVO_3$*, Phys. Rev. B **85**, 165103 (2012).

[2] J. Ferber, K. Foyevtsova, H. O. Jeschke, R. Valentí, *LDA+DMFT for organic molecular crystals: spectral and optical properties of κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Cl*, arXiv:1209.4466.