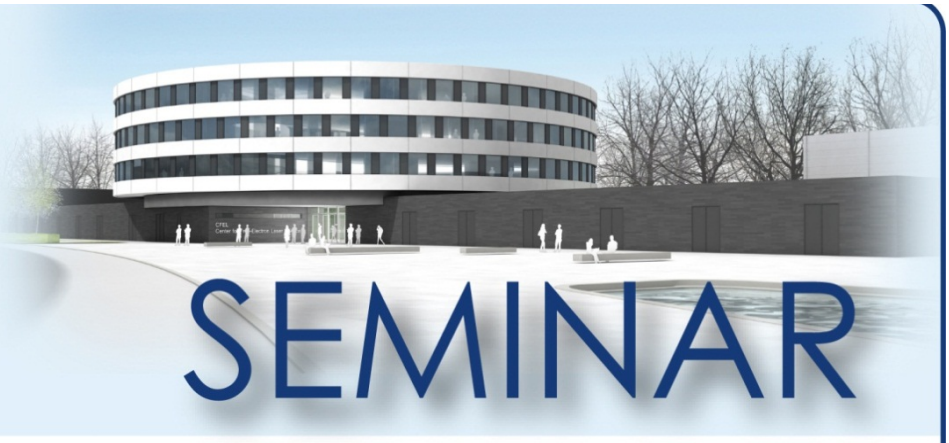
CFEL SCIENCE



SEMINAR

February 3, 2016 - 2:00 p.m.
CFEL-bldg. 99, seminar room IV

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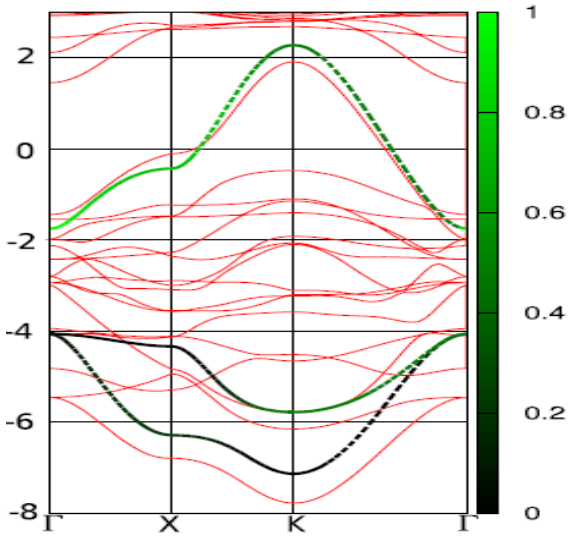
The role of dynamical screening in correlated materials

A physically motivated approach for studying the electronic structure of strongly correlated materials is to focus on a subspace of the full Hilbert space containing most of the relevant correlation effects. The reduction to a limited subspace results in an energy-dependent effective electron-electron interaction *U*. It was not until recently an impurity problem with dynamic *U* could be solved within dynamical mean-field theory (DMFT) using continuous-time quantum Monte Carlo technique. The energy dependence of *U* can have unexpected consequences. As an illustration, we consider La_2CuO_4, the prototype of high-temperature superconductor parent compounds. DMFT calculations on undoped La_2CuO_4 show the important role of dynamic *U*: starting from the local density band structure, the insulating state is not obtained when a static *U* calculated from first-principles is used. Analysis of *U* and the DMFT spectral functions leads to a new insight into the nature of the electronic structure of charge-transfer insulators to which La_2CuO_4 belongs.



Host: Angel Rubio – MPSD-CFEL Theory Department