Long-range Coulomb interactions and dynamical screening in correlated materials: a "GW+DMFT" perspective

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The field of electronic structure calculations for correlated materials has witnessed tremendous progress in recent years due to the development of combined electronic structure and many body techniques. We will show results on recent methodological developments in the field, concerning the description of dynamical screening effects in solids, and the combined GW and dynamical mean field scheme “GW+DMFT” [1].

Specifically, we argue that screening of the effective Coulomb interactions to be used in low-energy effective Hamiltonians for correlated materials gives rise to dynamical, that is, frequency-dependent interactions. We explore the consequences of these dynamical effects [2, 3], and show how they lead to additional renormalisations of the one-particle Hamiltonian [4]. Further, we present results of the first realistic implementations of the combined GW and dynamical mean field scheme "GW+DMFT" that fully include these dynamical screening effects [5, 6]. A model study of an extended Hubbard model [7, 8], as well as an ab initio study of systems of adatoms adsorbed on semiconducting surfaces [6] **(see also Poster by P. Hansmann)** demonstrate how the GW+DMFT scheme allows the backfolding of non-local Coulomb interactions into effective frequency-dependent local ones. Finally, we show that the GW+DMFT analysis of a seemingly simple benchmark system, the ternary transition metal oxide $SrVO_3$, leads to new surprises and a reinterpretation of spectroscopic data [5].

Work done in collaboration with the authors of the references below.

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