Dynamical screening effects in correlated materials from a dynamical mean field view: from "LDA+DMFT" to "GW+DMFT"

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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 density functional and many body theories. We will give a brief introduction to the combined density functional dynamical mean field scheme "LDA+DMFT", illustrated by examples of transition metal oxides [1].
Then, we will discuss recent methodological developments in the field. In particular, we will focus on ab initio calculations for the screened Coulomb interaction ("Hubbard U") [2]. We will argue that screening of the effective Coulomb interactions to be used in low-energy effective models for correlated materials gives in principle rise to dynamical, that is, frequency-dependent interactions. We explore the effects of these dynamical interactions [3,4], and show how they lead to additional renormalisations of the one-particle Hamiltonian [5].
Finally, we will present very recent results using a combination of Hedin's GW approximation and DMFT, both on an extended Hubbard model [6,7] and realistic materials [8,9].

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