Simulations of correlated materials:
non-local self-energies & dynamical screening

In recent years, much progress in electronic structure came from combining band theory approaches with many-body methods that solve the Hubbard model. Particularly successful is the merger "DFT+DMFT" of density functional theory and dynamical mean-field theory.
Yet, in the quest toward truly predictive calculations one needs to ascertain whether the "simplicity" of the Hubbard model and the approximations made when solving it, do sufficient justice to the complexity of the considered material.
In this talk I will discuss effects beyond standard DFT+DMFT: momentum-dependent self-energies, retarded and non-local interactions. Employing the so-called GW+DMFT approach as well as the ab initio dynamical vertex approximation (DGA), I will show that said effects are non-negligible even for compounds previously thought to be well understood within DFT+DMFT.