Dynamics and correlation functions in complex quantum materials

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The *ab initio* description of excitations and dynamics in crystals, thin-films molecules and nano-materials becomes a real challenge when correlations lead to states with large entanglement. At the same time many interesting phenomena are found when local correlations and delocalization both play a role. In those materials one can find, for example, high- temperature superconductivity, colossal magneto resistance, metal-insulator transitions, and many more exotic properties. Nanoclusters, surfaces, and interfaces provide us with the opportunity to combine and tune these fascinating properties, obtaining novel functionalities. Transition-metal ions with local correlations, interacting with the delocalized orbitals of an organic molecule, are often found as the active center in enzymes and catalysts, as beautifully realized in nature with the active role Mn atoms have in the fundamental process of photosynthesis.

In this talk I will illustrate, using several examples, how we work towards an *ab initio* method that can predict the ground-state, excitations as well as the dynamics of complex quantum materials with variable amount of correlations. For this we create models based on density functional theory and Wannier-functions. These models are solved using different methods, including a recently implemented scheme that merges ideas from density matrix renormalization group and quantum chemistry.