DFT+DMFT to correlated electronic structures: Recent developments and applications to iron-based superconductors

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Dynamical mean field theory (DMFT) has been widely used to study correlated systems which have open d or f shell and require treatment of correlation effects beyond static mean field theories such as the density functional theory (DFT). In this talk, I will first discuss recent developments in our group of a fully charge self-consistent implementation of DMFT into a full-potential all-electron DFT code, so-called DFT+DMFT, where the impurity problem is solved by a highly accurate continuous-time quantum Monte-Carlo solver. Then I will show some applications of our implementation of DFT+DMFT, taking the iron-based superconductors as examples, to compute various physical properties such as photo-emission spectroscopy, optical conductivity, spin and charge susceptibility, valence fluctuations, and so on. In the meantime, I will demonstrate that our DFT+DMFT provides a much better description of many experimental observable in comparison to the DFT. Hence the DFT+DMFT is a very promising tool to help us understand and design correlated functional materials.