Implementation of "charge-only-DFT"+U and k-resolved spectral function in DFT+DMFT.

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I present two developments that aim to improve the description of strongly correlated systems. First, I detail the implementation of the "charge-only-DFT"+U method proposed in Refs. [1]. It intents to improve the description of exchange in usual DFT+U. I show the benchmark of the implementation on magnetic effects on iron and I show the application of this method for properties of actinides [2]. Secondly, I present the implementation of **k**-resolved spectral function in DFT+DMFT. It requires the analytic continuation of the self energy from the imaginary frequency axis to the real frequency axis. I show the example of OmegaMaxent [3] which uses the Maximum Entropy method to do this continuation. I benchmark the implementation of spectral function in $SrVO_3$, and I show the application to α-cerium (cf Fig 1).

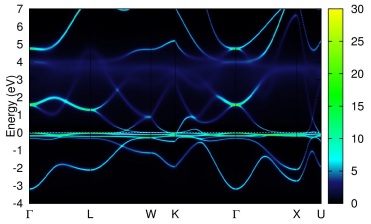

Figure 1: **k** resolved LDA+DMFT spectral function of α-cerium (U=6 eV)

References

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