Spectral properties of transition-metal pnictides: non-local exchange and dynamical screening

A. van Roekeghem

Centre de Physique Théorique, Ecole Polytechnique, CNRS-UMR7644, 91128 Palaiseau, France and Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China

We describe the effects of electronic correlations on the spectral properties of transition metal pnictides and chalcogenides. Our aim is to reproduce ab-initio and to interpret the results of angle-resolved photoemission spectroscopy (ARPES) measurements. The combination of the Local Density Approximation with Dynamical Mean Field Theory (LDA+DMFT) provides a good description for the overall quasiparticle renormalization. Nevertheless, on the example of BaCo2As2, we show that it is necessary to go beyond this approximation to describe accurately the Fermi surface and the magnetic properties. In particular, we establish the importance of non-local exchange and dynamical screening.

[1] A. van Roekeghem, T. Ayral, J.M. Tomczak, M. Casula, N. Xu, H. Ding, M. Ferrero, O. Parcollet, H. Jiang, and S. Biermann. Dynamical correlations and screened exchange on the experimental bench: spectral properties of the cobalt pnictide BaCo2As2. Phys. Rev. Lett., 113:266403, 2014.

[2] A. van Roekeghem and S. Biermann. Screened exchange dynamical mean field theory and its relation to density functional theory: SrVO3 and SrTiO3, EPL, 108:75003, 2014

[3] A. van Roekeghem, P. Richard, H. Ding and S. Biermann. Spectral properties of transition metal pnictides and chalcogenides: angle-resolved photoemission spectroscopy and dynamical mean field theory, C. R. Phys. 17 (1--2), 140—163, 2016

[4] A. van Roekeghem, P. Richard, X. Shi, S. Wu, L. Zeng, B. Saparov, Y. Ohtsubo, T. Qian, A.S. Sefat, S. Biermann and H. Ding. Tetragonal and collapsed-tetragonal phases of CaFe2As2 -- a view from angle-resolved photoemission and dynamical mean field theory, arXiv: 1505.00753, 2015

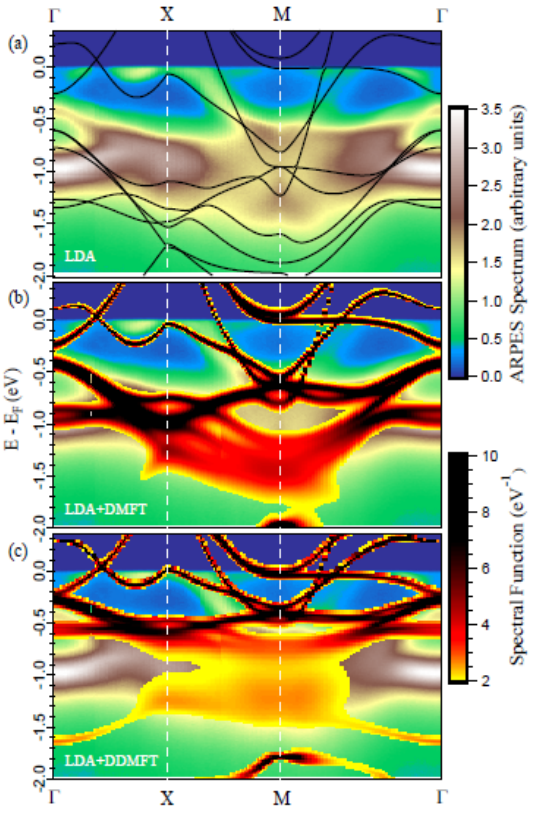

Figure 1: $BaCo_2As_2$ photoemission spectra, replotted from Ref. [35]. Superimposed are (a) the Kohn-Sham band structure of DFT-LDA (b) spectral function of standard LDA+DMFT [only those parts that exceed 2 states/eV are shown] (c) spectral function within LDA+DDMFT [same representation as in (b)].