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Accurate modeling of FeSe with screened Fock exchange and Hund's metal correlations

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The major role played by strong correlations in iron-based superconductors (IBSC) has been widely assessed, as pointed out by the successful predictions of local magnetic moments and mass differentiations in these materials. Nevertheless, cumulating evidence shows that local interactions alone cannot capture the finer details of their electronic structure, yielding Fermi pockets way too large when compared with experiments. This issue is most striking in FeSe, where single-site dynamical mean-field theory (DMFT) predicts Fermi pockets from five to six times larger than experiments [1], hampering the theoretical description of the related electronic instabilities. On general grounds, this deficiency has been related to the treatment of non-local interactions in the theoretical modeling [2]. I will show how the interplay between non-local exchange and local interactions is responsible for the main low-energy features of FeSe by means of hybrid-DFT + slave-spin mean-field calculations (HSE@SSMF). Within this framework, a net shrinking of the Fermi pockets accompanies an overall improvement of the quasiparticle properties, as documented by the comparison with angle-resolved photoemission spectroscopy (ARPES) and transport measurements [3].

[1] I. Leonov et al., PRL 115, 106402 (2015); M.D. Watson et al., PRB 95, 081106 (2017).
[2] L. Ortenzi et al., PRL 103, 046404 (2009); S. Bhattacharyya et al., PRB 102, 035109 (2020).
[3] T. Gorni et al., arXiv:2101.01692 (2021).

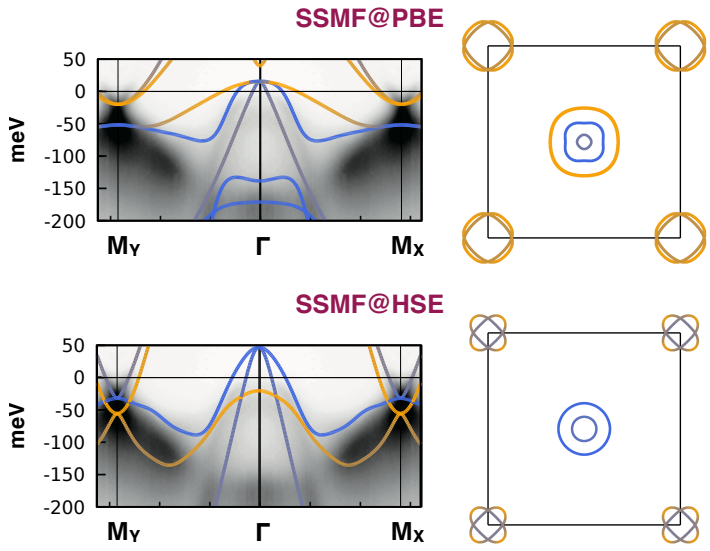

Figure 1 : Calculated band dispersion along the M_Y-Γ-M_X path (solid lines) on top of the corresponding ARPES dispersions (grey scale), and k_z=0-Fermi surface of FeSe, shown in the 2-Fe Brillouin Zone. The xy orbital weight is represented in a colour scale going from blue (zero weight) to orange (maximum weight).