25e Congrès Général de la Société Française de Physique

ID de Contribution: **234** Type: **Poster**

Exchange-Driven Red-Blue Shift in Iron Pnictides

Ten years after their discovery, the physics of iron-based superconductors (IBSC) has yet to be clarified, and a unified understanding of their behaviour is far from being reached. Even though the major role played by local correlations has been widely assessed, their inclusion alone is not able to reproduce some fundamental properties, most notably the size of electron and hole pockets of the Fermi surface [1,2,3]. In this regard, we study the effect of non-local interactions in the presence of strong local correlations within the IBSC XFe2As2 family (X=K,Ba,Rb,Cs), by means of Slave-Spin@Density-Functional Theory simulations. The inclusion of the non-local exchange interaction at the DFT level induces a red-blue shift in the Fermi pockets which betters the agreement with quantum oscillations and ARPES measurements. We also present the case of FeSe, in which the red-blue shift is not reproduced within our model, pointing towards interactions other than exchange as responsible for its peculiar behaviour.

[1] T. Terashima et al., J. Phys. Conf. Ser. 449, 012022 (2013).
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[3] M.D. Watson, et al., Phys. Rev. B 91, 155106 (2015).

Choix de session parallèle

Autres: Matière Condensée

Auteurs principaux: GORNI, Tommaso (ESPCI); Dr DE' MEDICI, Luca (ESPCI)

Orateur: GORNI, Tommaso (ESPCI)

Classification de Session: Séance Poster