Master 2: ***International Centre for Fundamental Physics***

INTERNSHIP PROPOSAL

Laboratory name: Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie
CNRS identification code: UMR 7590
Internship director' surname: HELLGREN
e-mail: maria.hellgren@upmc.fr Phone number: 01 44 27 52 23
Web page: http://www.impmc.upmc.fr/fr/equipes theorie_quantique_des_materiaux.html
Internship location: Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie (IMPMC), Sorbonne Université, Campus Jussieu, Paris
Thesis possibility after internship: YES (doctoral school EDPIF)
Funding: NO

Electron-phonon coupling in superconducting materials from advanced density functional approximations

The standard approach for treating the electron-phonon interaction is density functional theory (DFT) with so-called semi-local approximations [1]. During the past years it has become clear that this method is insufficient, and can fail dramatically in many systems of fundamental and technological interest such as high-temperature superconductors [2-4]. To solve the problem, an improved treatment of electronic correlation is needed. Indeed, recent works have shown that more advanced, fully nonlocal approximations in DFT tend to enhance the electron-phonon coupling, and in certain cases substantially increase the critical temperature of materials exhibiting unconventional superconductivity [3].

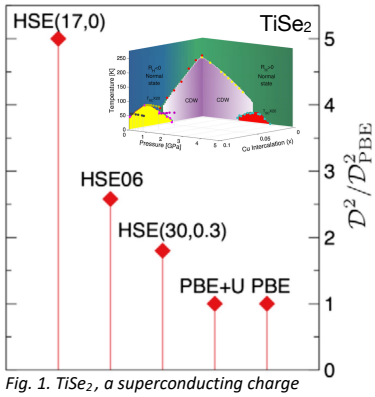


Fig. 1. $TiSe_2$, a superconducting charge density wave system. Enhancement of electron-phonon coupling going from simple DFT to more advanced approximations

In this project we will investigate and design nonlocal approximations based on diagrammatic many-body perturbation theory, able to simultaneously capture short and long range effects of the Coulomb interaction [5]. As a first application, we will study $TiSe_2$ an intriguing quasi-two-dimensional layered material where superconductivity competes with a charge density wave instability.

[1] J. P. Perdew and K. Schmidt, AIP Conf. Proc. 577, 1 (2001), [2] M. Lazzeri, C. Attaccalite, L. Wirtz, and F. Mauri, Phys. Rev. B 78, 081406(R) (2008), [3] Z. P. Yin, A. Kutepov, and G. Kotliar, Phys. Rev. X 3, 021011 (2013), [4] M. Hellgren, J. Baima, R. Bianco, M. Calandra, F. Mauri, L. Wirtz, Phys. Rev. Lett., 119 176401 (2017), [5] T.Pitts, D. Contant, M. Hellgren, Phys. Rev. B, 112, 085137 (2025)

Techniques/methods in use: Advanced density functional methods (RPA) and GW, development of electronic structure codes (Quantum ESPRESSO)

Please, indicate which speciality(ies) seem(s) to be more adapted to the subject:

Condensed Matter Physics: YES
Soft Matter and Biological Physics: NO
Quantum Physics: YES
Theoretical Physics: YES