

INTERNSHIP PROPOSAL

Laboratory name: Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie
 CNRS identification code: UMR 7590
 Internship director's 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)
 Funding: NO

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

The standard approach for treating the electron-phonon coupling from first principles is density functional theory within so-called semi-local approximations (LDA and GGAs). These methods fail, however, dramatically in systems with localised *d* or *f* electrons, failing to describe their insulating phases as well as their superconducting properties. Recent works have shown that improving the description of electronic correlation beyond semi-local approximations can strongly enhance the electron-phonon coupling, substantially increasing the critical temperature of certain materials exhibiting unconventional superconductivity [1,2].

In this project we will investigate why semi-local approximations fail and how to overcome their deficiencies with the design of fully nonlocal approximations able to simultaneously capture short and long range effects of the Coulomb interaction [3]. As an application, we will study TiSe₂, an intriguing *d* electron system where superconductivity competes with a charge density wave instability.

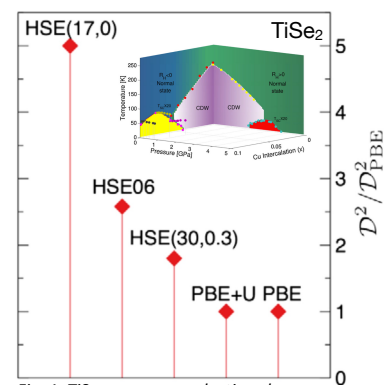


Fig. 1. TiSe₂, a superconducting charge density wave system. Enhancement of electron-phonon coupling going from simple DFT to more advanced approximations

[1] Yin et al, *PRX* 3, 021011 (2013), [2] Hellgren et al, *PRL*, 119 176401 (2017), [3] Pitts et al *PRB*, 112, 085137 (2025)

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

Condensed Matter Physics: YES
 Quantum Physics: YES

Soft Matter and Biological Physics: NO
 Theoretical Physics: YES