Electron-phonon interactions and magnetism in Fe-based superconductors

Thomas Frederiksen,[1] Bruno Rousseau,[2] Felix Yndurain[1,3]

1) DIPC – Donostia International Physics Center, Paseo Manuel de Lardizabal 4, 20018 Donostia-San Sebastián, Spain
2) Centro de Física de Materiales, CSIC-UPV/EHU, 20018 Donostia-San Sebastián, Spa in
3) Departamento de Física de la Materia Condensada, Universidad Autónoma de Madrid, Cantoblanco, 28049 Madrid, Spain.

Email: thomas_frederiksen@ehu.es

Since the recent discovery of superconductivity in layered Fe-based materials [1,2], with transition temperatures up to 55 K, enormous research efforts have been devoted to characterizing this new class of compounds. One of the most fundamental questions, namely the nature of the Cooper pairing mechanism responsible for superconductivity, is still intensely debated [3]. The coexistence of antiferromagnetic, non-superconducting phases and non-magnetic, superconducting phases depending on chemical doping have lead to theoretical studies exploring the importance of magnetic moments coupled to phonons for superconductivy [4,5,6].

Here we present a first-principles study of electron-phonon interactions and magnetism in $LaFeAsO_{1-x}F_x$ compounds. Our calculations are based on density functional theory as implemented in the SIESTA code [7]. We perform calculations using the virtual crystal approximation (VCA) as well as supercell calculations with F substitutional impurity atoms, and determine the electronic structure as a function of doping. Within a finite difference scheme [8] we further calculate the phonon properties and corresponding electron-phonon couplings to arrive at estimates for the effective electron-phonon coupling strength, conventionally labeled λ, as an average over the Fermi surface. By comparing trends for both non-magnetic and magnetic calculations we are able to quantify the importance of the detailed interplay between electron-phonon coupling and magnetism, as well as their role in superconductivity.

References

[1] Y. Kamihara, H. Hirmatsu, M. Hirano, R. Kawamura, H. Yanagi, T. Kamiya, and H. Hosono, J. Am. Chem. Soc. **128**, 10012 (2006).
[2] Y. Kamihara, T. Watanable, M. Hirano, and H. Hosono, J. Am. Chem. Soc. **130**, 3296 (2008).
[3] J. Paglione and R. Greene, Nature Physics **6**, 645 (2010).
[4] F. Yndurain and J. M. Soler, Phys. Rev. B **79**, 134506 (2009).
[5] L. Boeri, M. Calandra, I. I. Mazin, O. V. Dolgov, and F. Mauri, Phys. Rev. B **82**, 020506(R) (2010).
[6] F. Yndurain, arXiv:1009.4909.
[7] J. Soler, E. Artacho, J. Gale, A. Garcia, J. Junquera, P. Ordejon, and D. Sanchez-Portal, J. Phys.: Condens. Matter **14**, 2745 (2002).
[8] T. Frederiksen, M. Paulsson, M. Brandbyge, A.-P. Jauho, Phys. Rev. B **75**, 205413 (2007).