

Fe-based Superconductors: Structural Phase Transitions Tuned by Electronic Fluctuations

Myrsini Kaitatzi^{1,2,*}, Alexandros Deltsidis^{1,2}, Aleksandr Missiul³, Emil S. Bozin⁴,
Alexandros Lappas¹

¹ *Institute of Electronic Structure and Laser, Foundation for Research and
Technology-Hellas, Vassilika Vouton, 71110 Heraklion, Greece*

² *Department of Materials Science & Technology, University of Crete, Voutes,
71003 Heraklion, Greece*

³ *CELLS - ALBA synchrotron, 08290 Cerdanyola del Vallès, Catalonia, Spain*

⁴ *Condensed Matter Physics and Materials Science Department, Brookhaven
National Laboratory, Upton, NY 11973, USA*

In-depth studies elaborating on hybrid iron chalcogenide superconductors are of a great interest to the condensed matter physics community due to their intriguing behaviors arising from structural modifications and electronic correlations upon intercalation. Intercalation of the 8 K FeSe superconductor with organic molecules leads to a substantial enhancement of the critical temperature (T_c) up to 42 K [1]. In effect, in such hyper-expanded lattice superconductors subtle local distortions in their nanoscale environment are introduced (Fig.1). Our team has developed solvothermal synthesis pathways for $\text{Li}_x(\text{C}_5\text{H}_5\text{N})_y\text{Fe}_{2-z}\text{Se}_2$ intercalated samples with the purpose to investigate them with state-of-the-art synchrotron science tools. In one hand, high Q-resolution X-ray diffraction, over a broad temperature range (10-300 K) is utilized to shed light on possible structural phase transitions, taking place at the average level when the materials cross the T_c . Rietveld analysis suggests that their high- T_c relates to the tetragonal ThCr_2Si_2 -type structure. On the other hand, complementary high-energy synchrotron X-rays enable a wide-Q field of view, appropriate for total scattering insights [2]. When combined with pair distribution function (PDF) analysis, correlated local distortions, pertaining to the electronic active Fe-selenide layers, are identified as the outcomes of the electron donor moieties, accommodated in the interlayer space. The structural insights acquired from these studies are highly valuable in an effort to draw materials-design principles that help to optimize the electronic structure for attaining even higher T_c .

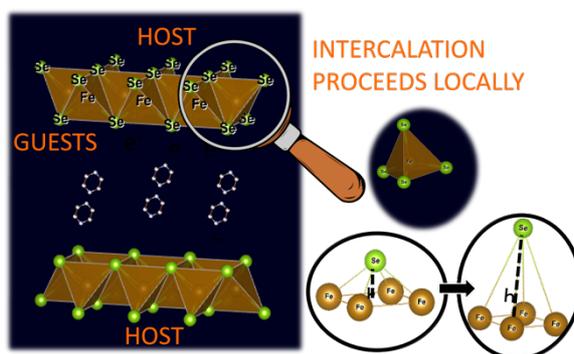


Figure 1: Interplay among lattice distortions doping and superconductivity.

References

- [1] A. Krzton-Maziopa et al., J. Phys.: Condens. Matter **30** 243001 (2018).
- [2] I.C. Berdiell et al., Inorg. Chem. **61**, 4350 (2022).

* myrsinik@iesl.forth.gr