

# Gap modulations within the unit cell in Fe-based superconductors

## 1. Observation of Cooper-pair density modulation state

Authors: Lingyuan Kong, Michał Papaj, Hyunjin Kim, Yiran Zhang, Eli Baum, Hui Li, Kenji Watanabe, Takashi Taniguchi, Genda Gu, Patrick A. Lee, and Stevan Nadj-Perge  
Nature **640**, 55 (2025)

## 2. Sublattice Dichotomy in Monolayer FeSe Superconductor

Authors: Cui Ding, Zhipeng Xu, Xiaotong Jiao, Qiyin Hu, Wenxuan Zhao, Lexian Yang, Kun Jiang, Jin-Feng Jia, Lili Wang, Jiangping Hu, and Qi-Kun Xue  
arXiv:2406.15239

## 3. Visualizing uniform lattice-scale pair density wave in single-layer FeSe/SrTiO<sub>3</sub> films

Authors: Yao Zhang, Lianzhi Yang, Chaoferi Liu, Wenhao Zhang, and Ying-Shuang Fu  
arXiv:2406.05693

## 4. Observation of Superconducting Pair Density Modulation with Lattice Unit Cell

Authors: Tianheng Wei, Yanzhao Liu, Wei Ren, Zhen Liang, Ziqiang Wang, and Jian Wang  
Chinese Physics Letters **42**, 027404 (2025)

*Recommended with a Commentary by Daniel F. Agterberg ,  
University of Wisconsin - Milwaukee*

Fe-based superconductors have fascinated the quantum materials community because of their interplay of magnetic, nematic, and superconducting electronic orders [1, 2]. Lately, the emphasis in this community has shifted to Fe-chalcogenides, where important open questions, such as the pairing symmetry of monolayer FeSe on SrTiO<sub>3</sub> (STO), still remain. Scanning tunneling microscopy/spectroscopy (STM)/STS has allowed new insight into these questions. Specifically, as reported in the four papers mentioned above [3, 4, 5, 6], variations in the superconducting order within the crystallographic unit cell have been observed. Understanding these variations suggests the development of new electronic orders. In the following, we will focus on the first two papers [3, 4]. The other two papers [5, 6] give results that are qualitatively similar, but differ in some details.

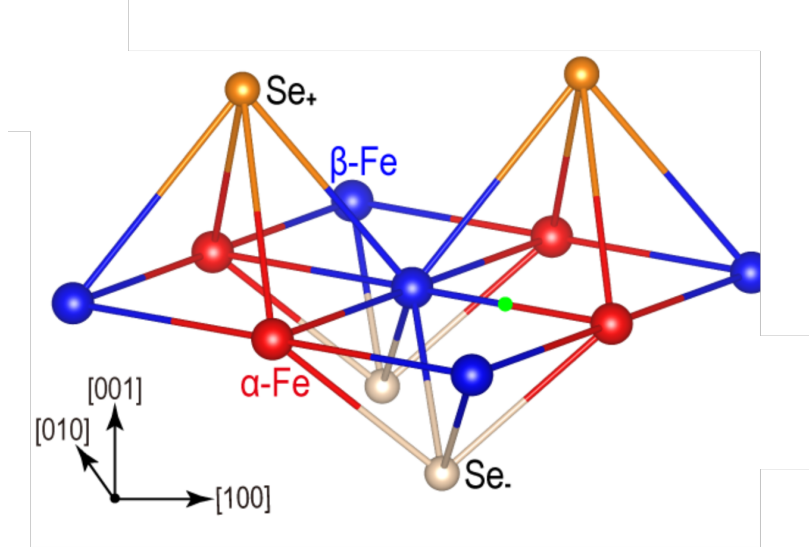


Figure 1: Structure of the unit cell in the FeSe-based materials discussed here. The two distinct Fe-atoms in the unit cell are labeled  $\alpha$  and  $\beta$ . Adapted from [4].

Before a discussion of Refs. [3, 4], it is useful to highlight two relevant properties of these FeSe-based superconductors. The first is the structure of the crystallographic unit cell. This is shown in Figure 1, key is the existence of two Fe in each unit cell, here labeled Fe- $\alpha$  and Fe- $\beta$ . These two Fe atoms are related by two symmetries: a mirror glide symmetry (a mirror reflection through the [001]-axis followed by half a translation vector); and a four-fold rotation about an axis running through one of the Se sites. The second property is the electronic structure of these materials. In Fe-based superconductors, both electron and hole pockets often appear. The hole pockets are near the center of the Brillouin zone (the  $\Gamma$  point), while the electron pockets near the corner of the Brillouin zone (the  $M$  point). Interestingly in Paper 1, in which thin exfoliated flakes of bulk  $\text{FeTe}_x\text{Se}_{1-x}$  are examined, only hole pockets near the  $\Gamma$  point have been observed [3]. In Paper 2, which examines monolayer FeSe grown on STO, it is well known that only electron pockets near the  $M$  point appear [1, 2]. In spite of this difference in the electronic structure, both papers report STM/STS measurements in the superconducting state that differ on the two Fe atoms within the unit cell. However, as described in detail in the following paragraph, the manner in which the STS/STM spectra on each Fe site differ is not the same for the two materials.

For Paper 1 [3], a representative plot of  $dI/dV$  on the two Fe sites is shown in Figure 2a. The key here is that the spectrum on each site is approximately particle-hole symmetric and reveals a nodeless gap that is of different magnitude on the two Fe sites. The authors of Paper 1 [3] call this a pair density modulation (PDM). For Paper 2, the  $dI/dV$  spectra for the two Fe-sites are shown in Figure 2b. Here, the two Fe sites again exhibit a nodeless gap; in this case, the gap magnitudes are similar, but the spectra for each Fe site are approximately related by a particle-hole transformation (that is, by changing the sign of the bias on the x-axis in Fig. 2b). The authors of Paper 2 [4] call this sublattice dichotomy. The measurements in [3, 4, 5, 6] likely represent the first observation of the variation of the superconducting order within a single crystallographic unit cell. As described below, understanding the

origin of these intra-unit cell site variations provides nontrivial information about electronic interactions in these materials.

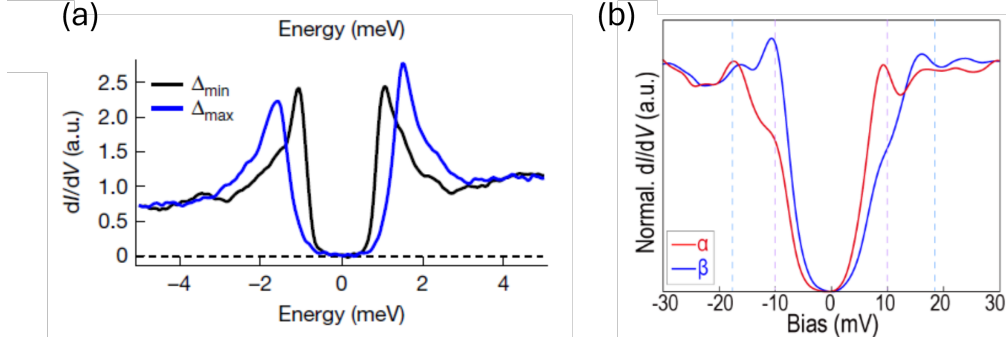


Figure 2: The  $dI/dV$  curves for the two Fe sites in the unit cell for the materials in papers 1 and 2. (a) Representative  $dI/dV$  curves for a thin exfoliated flake of bulk  $\text{FeTe}_x\text{Se}_{1-x}$ , revealing a pair density modulation (a different size gap on the two Fe sites). Adapted from Ref. [3] (b) Representative  $dI/dV$  curves for monolayer Fese on STO revealing a sublattice dichotomy (the two Fe sites are related by a particle-hole symmetry in which the bias is reversed). Adapted from Ref. [4].

Although new from an experimental perspective, the spatial variation of superconducting order within the crystallographic unit cell has been discussed theoretically. In 1985, P.W. Anderson suggested that this must occur in odd-parity heavy-fermion superconductors [7]. A microscopic description of such an odd-parity state was subsequently developed by Yoshida, Sigrist, and Yanase [8] and later argued to be realized in  $\text{CeRh}_2\text{As}_2$  [9]. In Kagome superconductors, it was realized that a superconducting state with a gap that differs on the three Kagome sites in the unit cell is a likely pairing state [10]. In these examples, the spatial variation of the gap in the unit cell is a consequence of pairing interactions that define the gap symmetry. For example, consider an interaction driven odd-parity superconductor in a material with two atoms in the crystallographic unit cell. If these two atoms are inversion symmetry partners, then the odd-parity symmetry condition requires that the gap is of opposite sign on these two atoms [7]. In Papers 1 and 2 [3, 4], the explanations provided suggest a different origin: symmetry breaking, possibly driven by electron correlations in the normal state.

In Paper 1, if it is assumed that the superconductor has  $s$ -wave symmetry, then superconductivity cannot be the source of the different spectra on the two Fe sites. The only possibility then is that there is a symmetry breaking that causes the two Fe sites to be inequivalent. Since STM is a surface probe, and the surface breaks mirror symmetry, a likely candidate is the glide mirror symmetry. However, there is still a 4-fold symmetry that remains that relates the two Fe sites, so the breaking of the mirror glide symmetry is not sufficient to cause the asymmetry. The authors of Paper 1 argue that the 4-fold symmetry is broken through either the appearance of a nematic order with a  $x^2 - y^2$  symmetry or through the appearance of a  $d_{x^2-y^2}$  gap in addition to the  $s$ -wave gap. From a symmetry perspective these explanations are equivalent; both imply the existence of a nematic order (either of intrinsic origin or driven by superconductivity). Interestingly, this nematic order

is not the same as that usually observed in Fe-based superconductors [2], which has a  $xy$  symmetry. Indeed, modeling the presence of a  $xy$  nematic order is not able to reproduce the observed pair density wave modulation [3]. The authors of Paper 1 provide additional evidence for the existence of this  $x^2 - y^2$  nematic order by showing that the pair density modulation has a domain structure consistent with such a nematic order.

In Paper 2, the interpretation appears quite different from that of Paper 1. Here again, a  $s$ -wave superconducting state is assumed, specifically a sign-changing  $s$ -wave order on the two electron pockets near the M point. It is argued that the substrate induces a symmetry breaking that allows an odd-parity superconducting order to appear, and the coexistence of the  $s$ -wave order with the odd-parity order gives rise to the sublattice dichotomy [4]. It is important in the theory that the odd-parity order is interband, and if this is not the case, the sublattice dichotomy vanishes [4]. However, this interband nature makes the odd-parity state unlikely to be intrinsically stabilized, and hence it should be induced by a symmetry breaking, likely due to the STO substrate, that exists in the normal state. Specifically, how this symmetry breaking leads to the appearance of the odd-parity state remains an open question. Nevertheless, the sublattice dichotomy seems to require an unusual gap structure, and a substrate-induced odd-parity state is a candidate that explains the data.

In both Papers 1 and 2, the interpretation of the spatially varying superconducting order within the crystallographic unit cell required new physics: a new nematic order in Paper 1 and a new, likely substrate-induced, odd-parity pairing in Paper 2. This suggests that measuring the variations of superconducting order within the unit cell provides a valuable new probe for correlated quantum materials.

## References

- [1] A. Kreisel, P. J. Hirschfeld, and B. M. Andersen, *Symmetry* **12**, 1402 (2020).
- [2] R.M. Fernandes *et al.*, *Nature* **601**, 25 (2022).
- [3] L. Kong *et al.*, *Nature* **640**, 55 (2025).
- [4] C. Ding *et al.*, arXiv:2406.15239 (2024).
- [5] Y. Zhang *et al.*, arXiv:2406.05693 (2024)
- [6] T. Wei *et al.*, *Chinese Phys. Letters* **42**, 027404 (2025).
- [7] P.W. Anderson, *Phys. Rev. B* **32**, 499(R) (1985).
- [8] T. Yoshida, M. Sigrist, and Y. Yanase, *Phys. Rev. B* **86**, 134514 (2012).
- [9] S. Khim, J.F. Landaeta, J. Banda, N. Bannor, M. Brando, P.M.R. Brydon, D. Hafner, R. Kuchler, R. Cardoso-Gil, U. Stockert, A.P. Mackenzie, D.F. Agterberg, C. Geibel, and E. Hassinger, *Science* **373**, 1012 (2021).
- [10] T. Schwemmer *et al.*, *Phys. Rev. B* **110**, 024501 (2024).