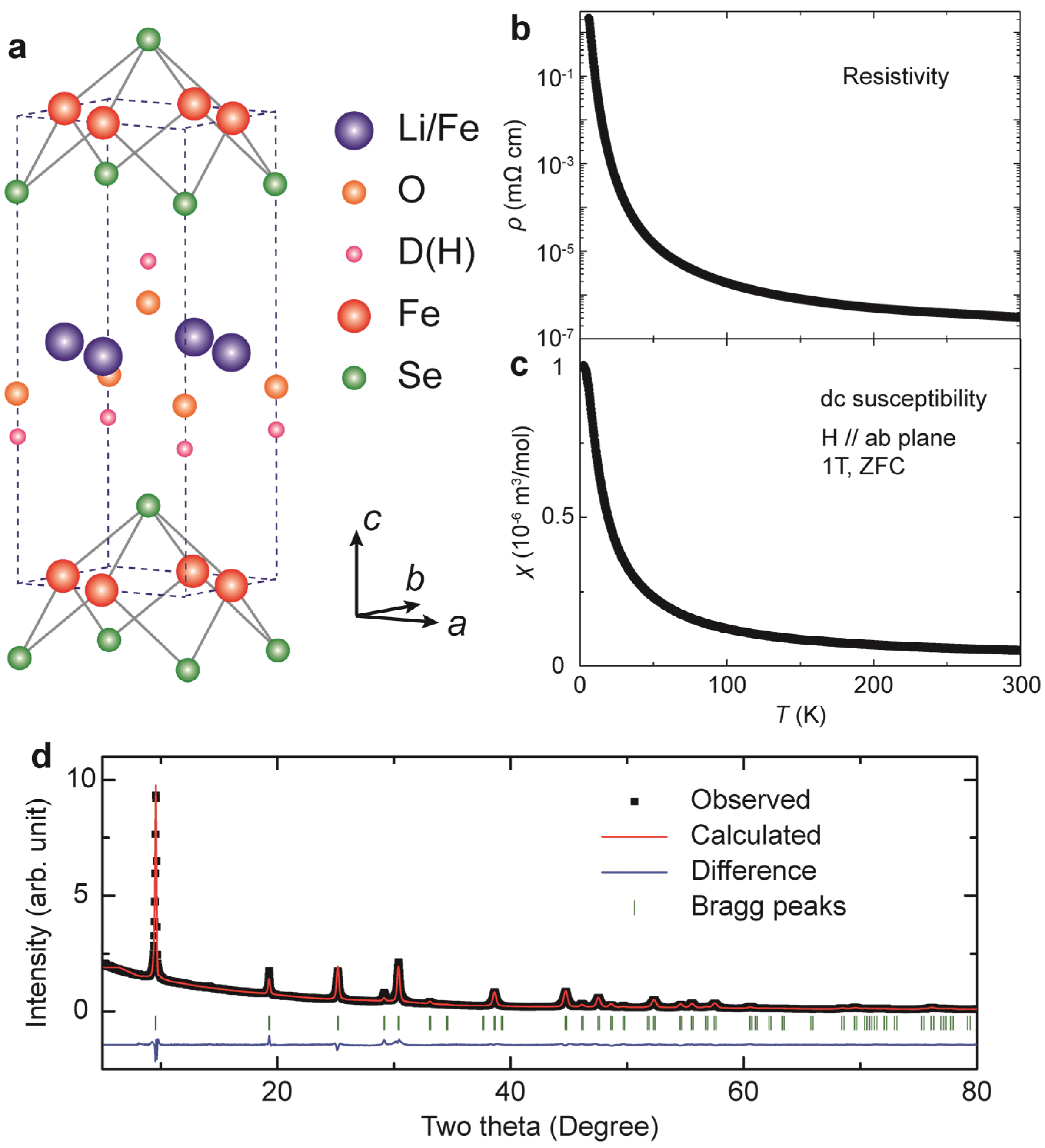
Spin excitations in the parent phase of a heavily electron-doped iron-based superconductor

Hongliang Wo[1,2], Bingying Pan[3], Die Hu[1], Yu Feng[4], A. D. Christianson[5], Jun Zhao*[1,6,2,7]

[1]State Key Laboratory of Surface Physics and Department of Physics, Fudan University, Shanghai, 200433, China [2]Shanghai Qi Zhi Institute, Shanghai, 200232, China [3]School of Physics and Optoelectronic Engineering, Ludong University, Yantai, Shandong 264025, China [4]Spallation Neutron Source Science Center, Dongguan 523803, China [5]Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA [6]Institute of Nanoelectronics and Quantum Computing, Fudan University, Shanghai 200433, China [7]Shanghai Research Center for Quantum Sciences, Shanghai 201315, China

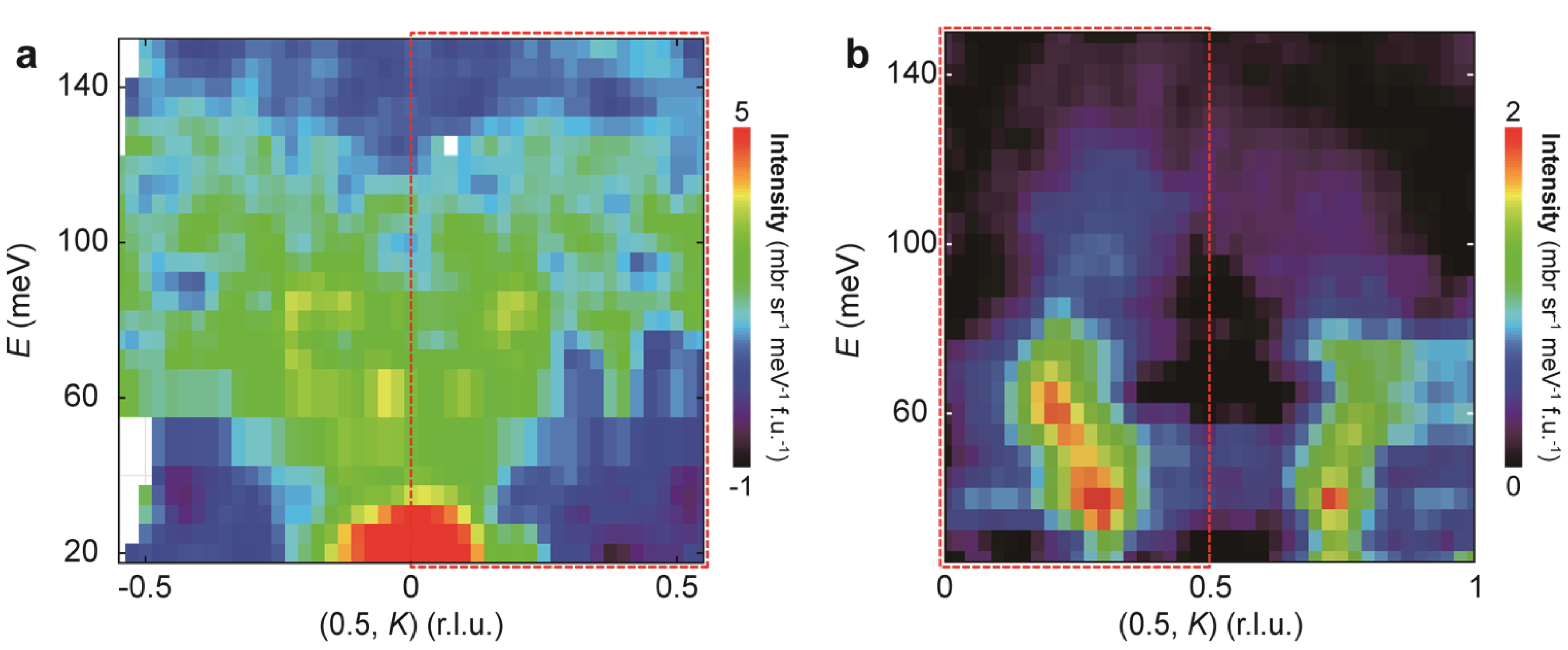
Abstract Heavily electron-doped iron selenide superconductors have attracted enormous attentions for their relatively high transition temperatures and unique electronic structures with no hole Fermi surfaces. Elucidating the nature of magnetism of their parent compounds is a key step to establish a right basis for relevant theories. Here, we present inelastic neutron scattering measurements of spin excitations in insulating $Li_{1-x}Fe_xODFeSe$, which is considered as the parent compound of this system. We show that the spin excitations stem from the stripe wave vector (π, 0) and disperse outward with increasing energy, exhibiting a V-shaped dispersion and reaching the band top at around 150 meV. This is distinct from its superconducting counterpart with an hourglass dispersion arising from the Néel wave vector (π, π). Our results highlight the importance of localized magnetism and strong correlation effects in iron selenides.

Lattice structure and sample characterization of non-superconducting $(Li_{0.8}Fe_{0.2})ODFeSe$



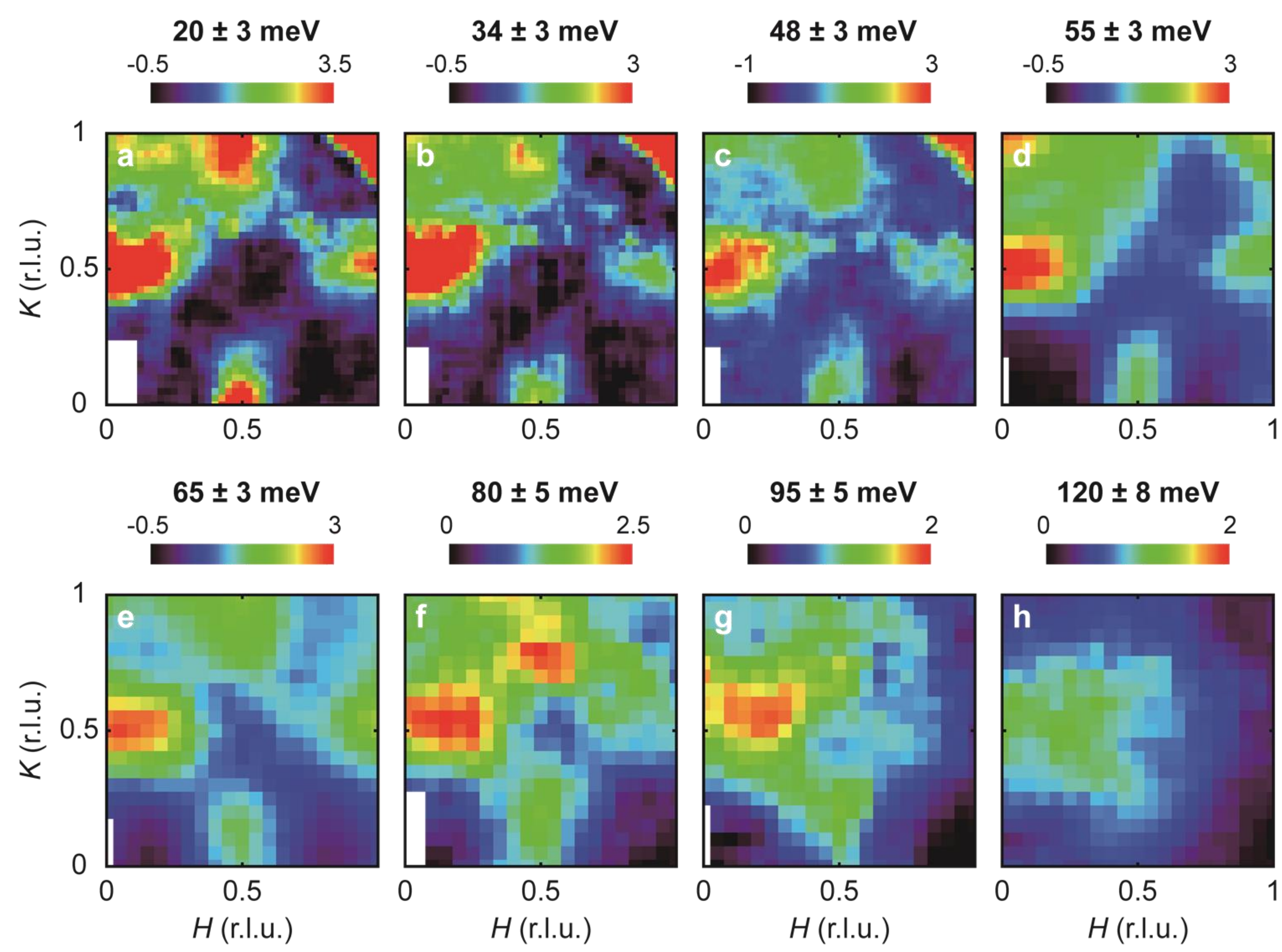
(a) Schematic diagram of $(Li_{1-x}Fe_x)ODFeSe$ crystal structure. **(b)** Resistivity measurement indicating the semiconducting nature of the parent compound. **(c)** Dc magnetic susceptibility of the insulating $(Li_{1-x}Fe_x)ODFeSe$ exhibits a Curie-Weiss behavior. No long-range magnetic order is observed down to 2 K. **(d)** X-ray powder diffraction pattern using grinded single crystals shows no detectable impurities.

Spin excitations along *K* direction: Comparison with optimal-doped compound



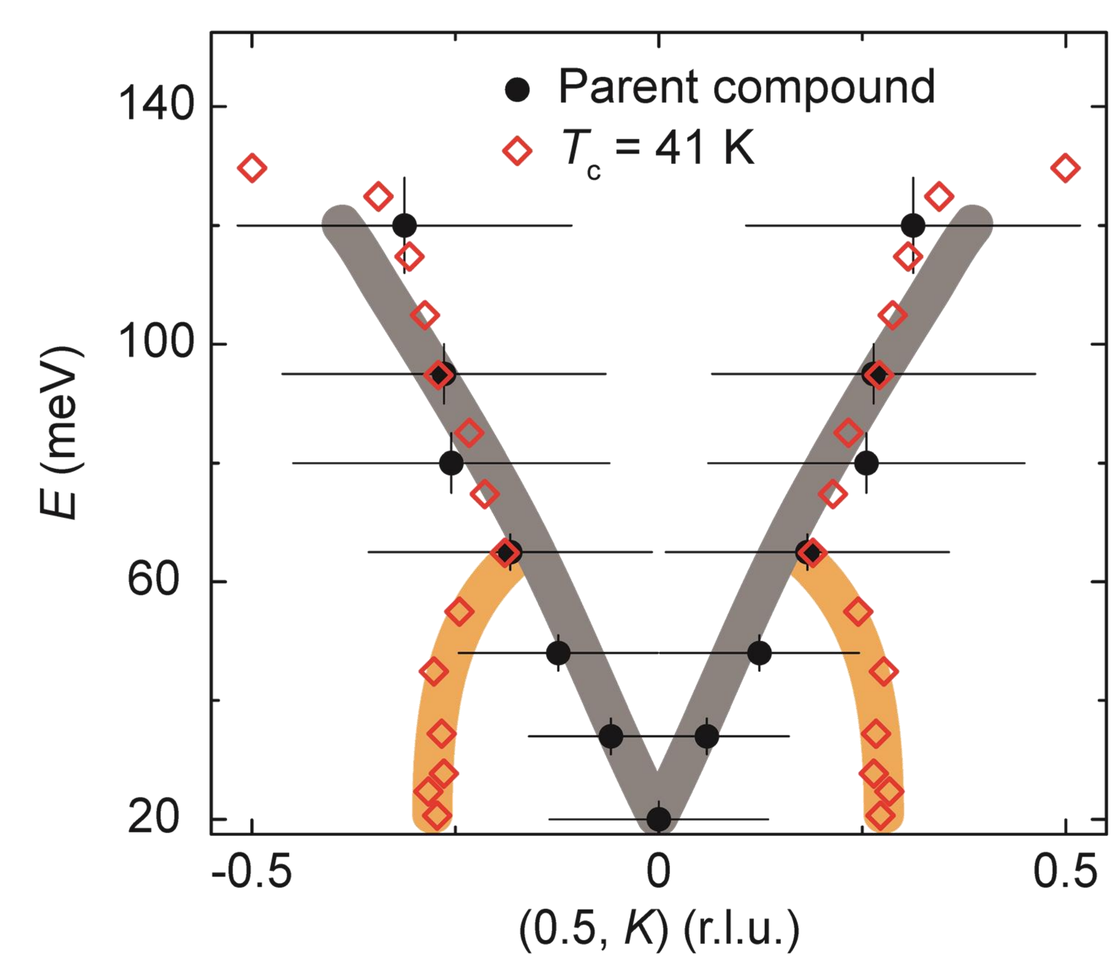
Background-subtracted spin excitation spectrum projected on the (0.5, *K*) direction in **(a)** non-superconducting and **(b)** optimally-doped $(Li_{1-x}Fe_x)ODFeSe$ at T = 5 K. The red dashed boxes correspond to the same region in the **Q**-*E* space.

Momentum dependence of the spin fluctuations in (*H*, *K*) plane at 5 K



Background subtracted constant-energy images at indicated energies in $(Li_{1-x}Fe_x)ODFeSe$. The data was collected at T = 5 K. The spin excitations stem from (0.5, 0) and equivalent positions (in 1-Fe notation) at low energies. With energy increasing, the stripe-type spin excitations disperse outward transversely to the reduced q. The signals finally merge around (0.5, 0.5) as the zone boundary.

Q-*E* relationship extracted from Gaussian fitting: An overplot



Overplot of **Q**-*E* dispersion of the spin excitations in non-superconducting and optimally-doped $(Li_{1-x}Fe_x)ODFeSe$. The dispersions of the two compounds highly coincide at high energy. Below 60 meV, the dispersion in optimally-doped one deviates from V-shape forming the twisted “hourglass” behavior.

Summary

- Spin excitations in non-SC phase of $(Li_{1-x}Fe_x)ODFeSe$ exhibit a V-shaped dispersion, in contrast to the “hourglass” one in optimally-doped compound.
- The low-energy spin excitations in SC sample could have strong interplay with the Fermi surface and superconductivity, all of which originate from the itinerant electrons.

References

[1] B. Y. Pan *et al.*, Nat. Commun. 8, 123 (2017).
[2] H. L. Wo *et al.*, in submission.