Origin of superconductivity and nature of correlations in extremely hole-doped iron-based superconductors under pressure

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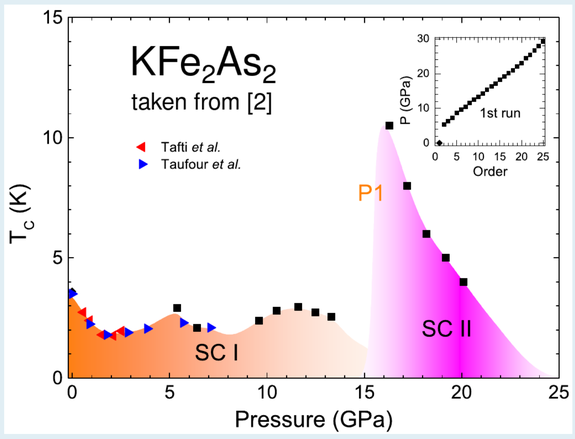
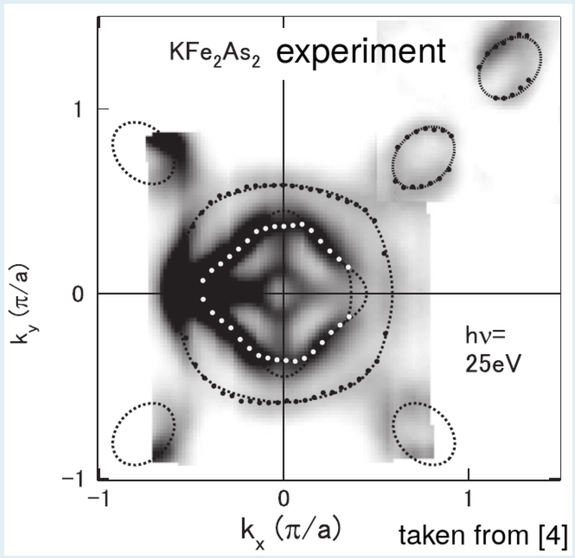
Superconductivity in AFe_2As_2 (A=K,Rb,Cs)

- $T_c \leq 3.4$ K superconductors at ambient pressure
- unusual V-shaped dependence of T_c on pressure below $P = 5$ GPa [1]
- collapsed phase of KFe_2As_2 with $T_c \sim 12$ K at $P = 16$ GPa [2,3]
- symmetry of superconducting order parameter unclear, $s\pm$ or d-wave?

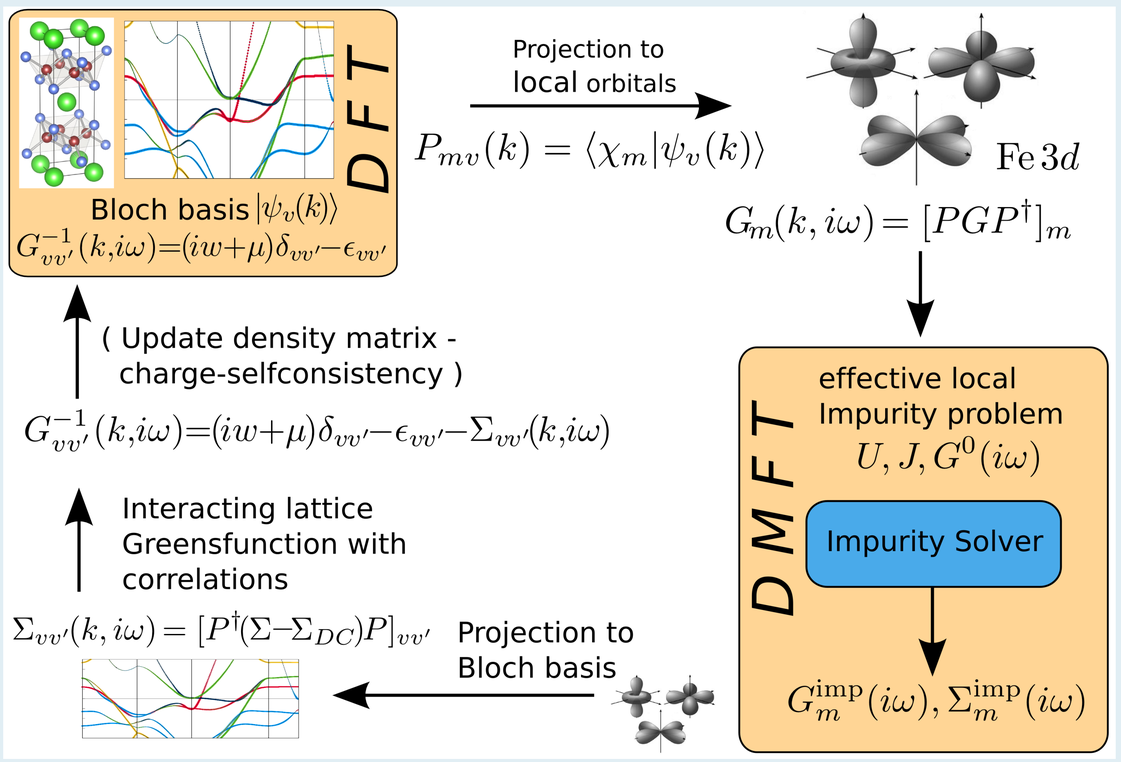


Electronic structure of KFe_2As_2 at ambient pressure

- Fe is nominally in $3d^{5.5}$ state, strongly hole-doped
- ARPES shows large hole cylinders with flower-shape on the inner pockets [4]
- no flower-shape in DFT, wrong relative pocket sizes
- effective masses of up to $m^* = 18m_e$ in de Haas-van Alphen experiment [5]
- very poor agreement between DFT and quantum oscillation frequencies



Implementation of the LDA+DMFT loop



- DFT calculation with WIEN2k, projective Wannier functions
- continuous-time quantum impurity solver (CTHYB) from ALPS
- full charge self-consistency
- stochastic analytic continuation

LDA+DMFT for KFe_2As_2 at ambient pressure

- full charge self-consistency is crucial
- spectral function agrees very well with ARPES
- agreement with quantum oscillations is improved, but not perfect
- strong orbital dependent mass renormalization
- very incoherent spectral weight at room temperature
- published as New J. Phys. **16**, 083025 (2014)

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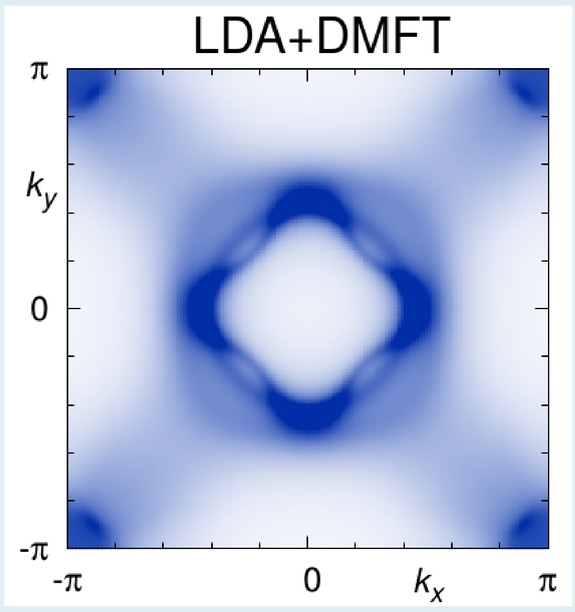
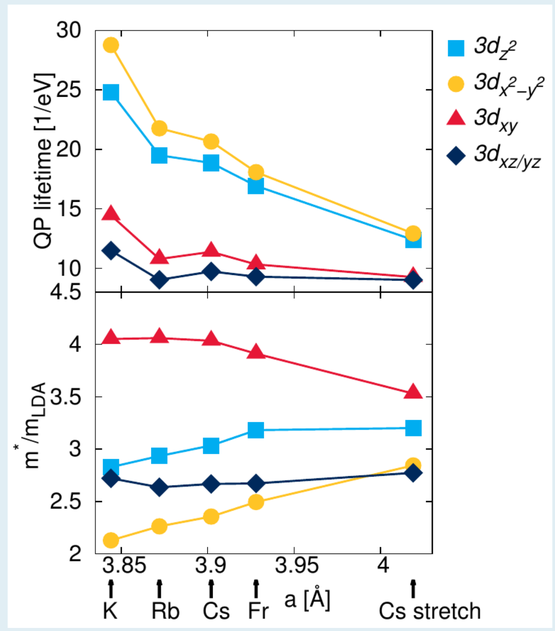
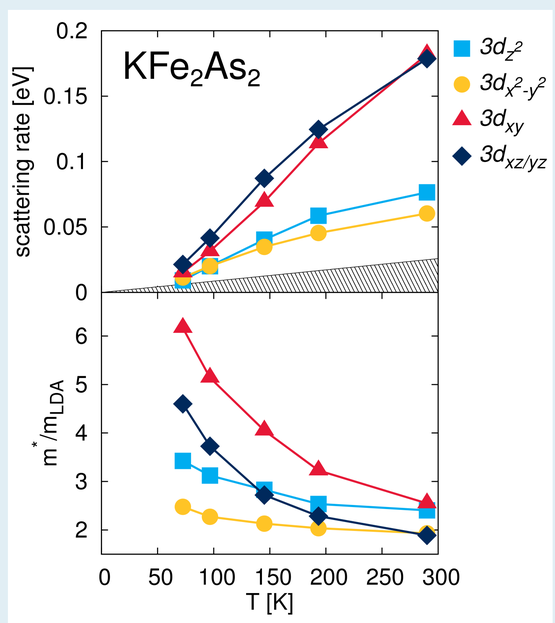


Microscopic nature of correlations in AFe_2As_2 (A=K,Rb,Cs,Fr)

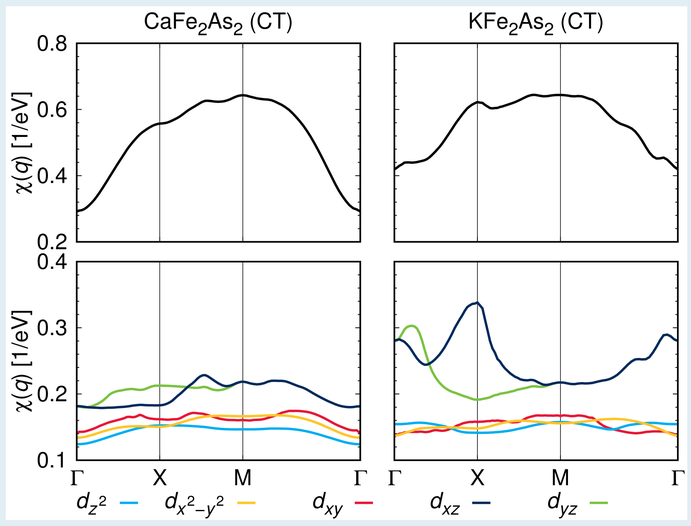




- larger alkali atoms act like negative pressure
- hole-doped pnictides are deep in bad metal regime
- Hund's rule coupling determines correlation strength
- behavior different from orbital-selective Mott transition
- nevertheless very large mass enhancements
- coherence scale of ~ 50 K
- preprint available as arXiv:1507.07914

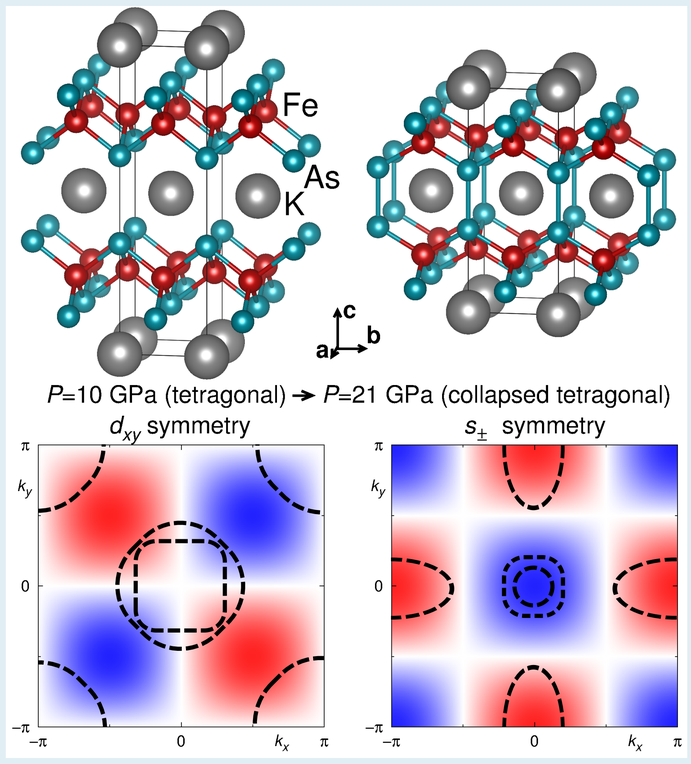
Electronic structure of high-pressure collapsed tetragonal KFe_2As_2

- previously known collapsed phases feature electron pockets only
- pressure dramatically reduces correlation strength
- Fermi surface is the same in LDA and LDA+DMFT
- in KFe_2As_2 also hole-pockets in Brillouin zone center due to hole-doping
- usual $(\pi, 0)$ nesting is present, strong peak in spin-susceptibility near X-point



Superconductivity in KFe_2As_2 under high pressure

- Lifshitz transition at structural collapse
- calculate superconducting order parameter in RPA spin-fluctuation approach
- transition from d-wave to $s\pm$ under high pressure predicted
- published as PRB **91**, 140503(R) (2015)



References

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