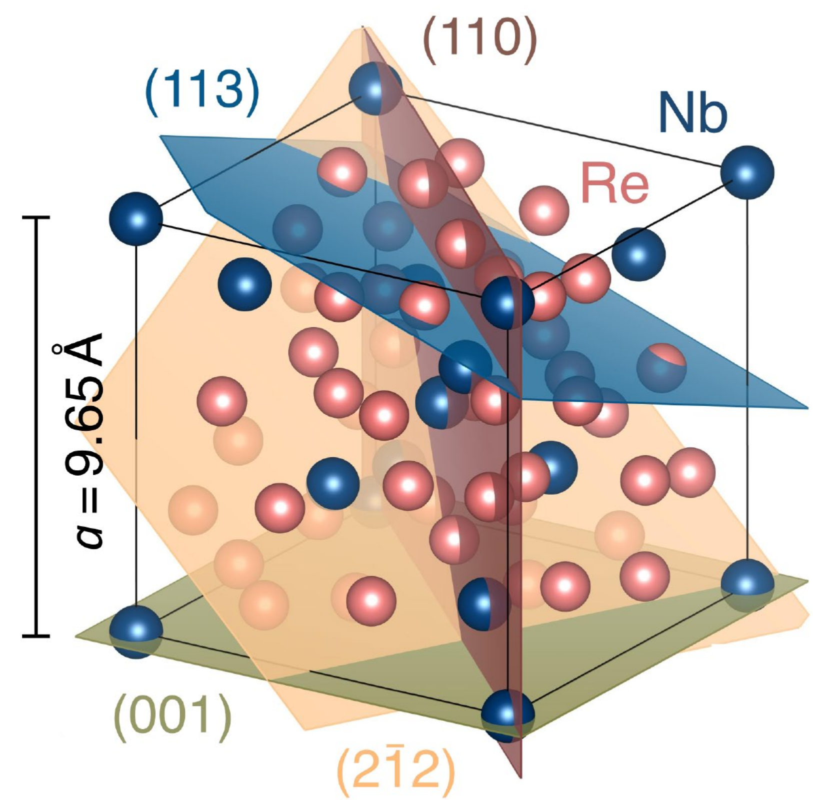
Q-M&S Correlated Quantum Materials & Solid State Quantum Systems

SFB 1432

Universität Konstanz

arXiv:2606.04742
[cond-mat.supr-con]

Spectroscopic evidence for nodal pairing symmetry in the NCS $Nb_{18}Re_{82}$



TIDES 2026

M. Strohmeier, A. Smolyanyuk, K. Held, M. Smidman, G. Balakrishnan, W. Belzig, E. Scheer & A. Di Bernardo

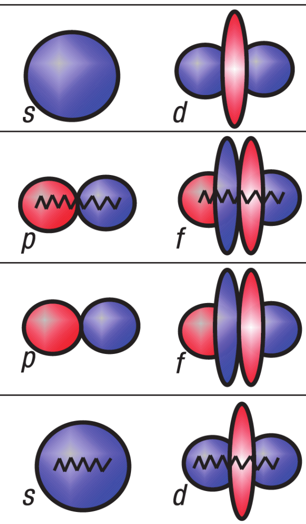
Pairing symmetry

momentum · spin · frequency

Pair amplitude $$F_{ss'}(\mathbf{k},\omega) = \langle c_{-\mathbf{k}s}(-\omega)\, c_{\mathbf{k}s'}(\omega)\rangle = \phi(\mathbf{k})\, \chi_{ss'}\, f(\omega)$$

Pauli exclusion principle must be fulfilled!

Spin	Frequency	Momentum
Singlet (odd)	Even	Even
$\uparrow\downarrow - \downarrow\uparrow$	Odd	Odd
Triplet (even) $\uparrow\uparrow$ $\downarrow\downarrow$	Even	Odd
$\uparrow\downarrow + \downarrow\uparrow$	Odd	Even



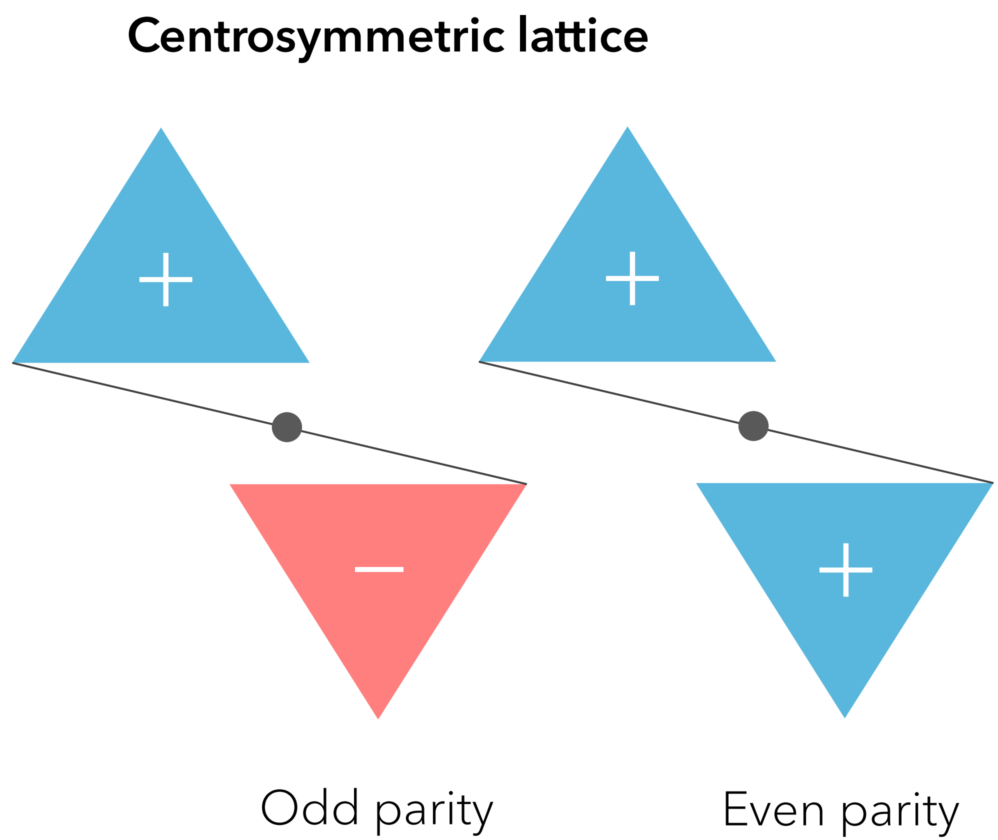
M. Eschrig and T. Löfwander, Nature Physics **4**, 138 (2008)

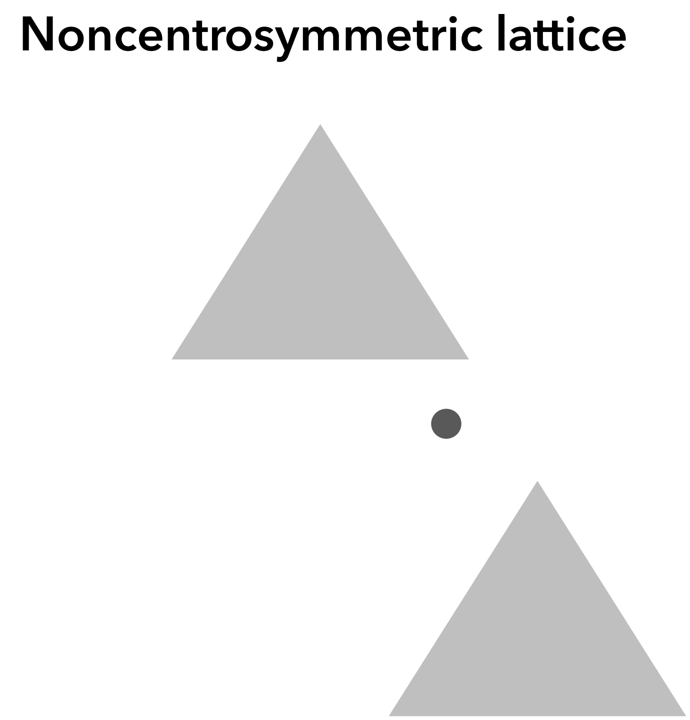
$\Longrightarrow$ Superconducting states beyond spin-singlet, s-wave pairing

- Odd-frequency pairing
- Anisotropic (nodal) pairing
- Spin-triplet pairing

...

Noncentrosymmetric superconductor (NCS)





Parity is not a good quantum number!

Noncentrosymmetric superconductor (NCS)

Crystal with lack of inversion symmetry

Microscopic electric field gradients on the atomic scale

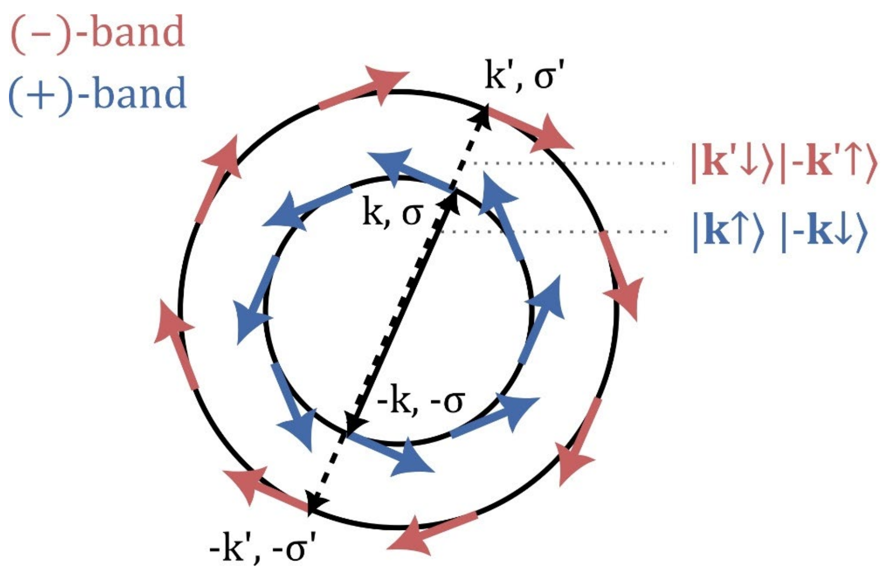
= (relativistic effects $\mathbf{B} \propto \mathbf{v} \times \mathbf{E}$)

Electron experiences a momentum-dependent magnetic field

ASOC (Rashba type) creates spin splitting of the electronic bands

Canonical pairing state in NCS

Two-dimensional Fermi surface with Rashba-type spin splitting



Two-component order parameter

$$\hat{\Delta}(\mathbf{k}) = \left[\Delta_s \psi(\mathbf{k}) + \Delta_t \mathbf{d}(\mathbf{k}) \cdot \hat{\boldsymbol{\sigma}}\right] i\hat{\sigma}_y$$

$\psi(\mathbf{k})$: scalar function (even parity)

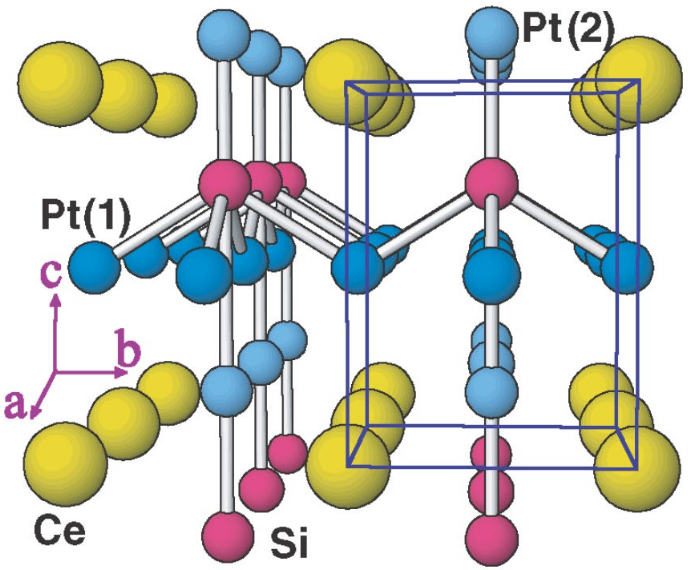
$\mathbf{d}(\mathbf{k})$: vector function (odd parity)

Pairing configurations: **admixture** of spin-singlet and spin-triplet states

$$|\mathbf{k}\uparrow\rangle|-\mathbf{k}\downarrow\rangle = \underbrace{\frac{1}{2}\left(|\mathbf{k}\uparrow\rangle|-\mathbf{k}\downarrow\rangle - |\mathbf{k}\downarrow\rangle|-\mathbf{k}\uparrow\rangle\right)}_{\text{Singlet state}} + \underbrace{\frac{1}{2}\left(|\mathbf{k}\uparrow\rangle|-\mathbf{k}\downarrow\rangle + |\mathbf{k}\downarrow\rangle|-\mathbf{k}\uparrow\rangle\right)}_{\text{Triplet state}}$$

Prototype heavy-fermion NCS $CePt_3Si$

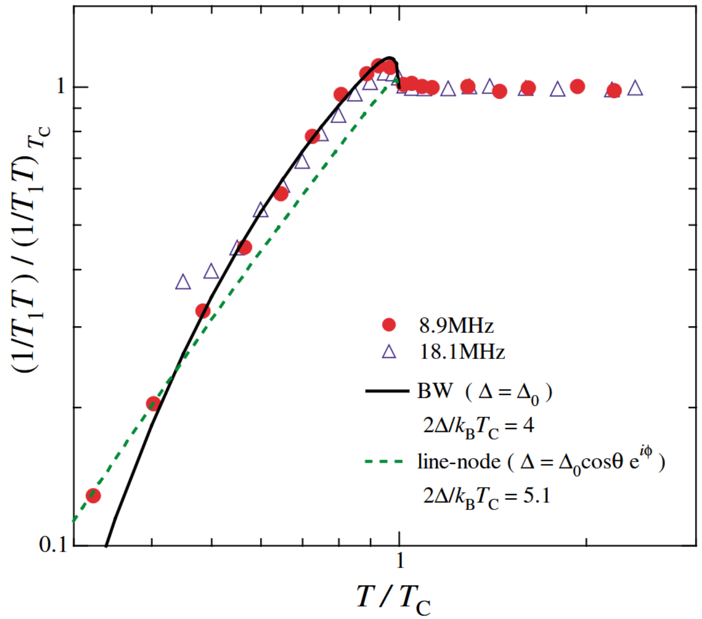
P4mm (tetragonal), E_{ASOC} ~ 200meV



Bauer *et al.*, Phys. Rev. Lett. **92**, 027003 (2004)

^{195}Pt-NMR Study of the spin-lattice relaxation rate $1/T_1$

Early interpretation (2006): Hints for spin-triplet pairing and mixed-parity order parameter in $CePt_3Si$



Yogi *et al.*, Phys. Rev. Lett. **93**, 027003 (2004)
Yogi *et al.*, J. Phys. Soc. Jpn. **75**, 013709 (2006)

Coexistence of AFM and SC phases

- Critical temperature T_c = 0.7 K
- Antiferromagnetic order at T_N = 2.2 K

Experimental evidence for parity mixing

- First non-centrosymmetric heavy-fermion (HF) compound $CePt_3Si$
- Impact of the ASOC on the nodal gap studied in $Li_2(Pd_{1-x}Pt_x)_3B$
- Several examples with strong ASOC without evidence for parity mxing (many weakly correlated e-ph-driven NCS with s-wave symmetry!)

State of knowledge

Parity mixing (with significant triplet component) requires

ASOC + Correlation effects

F. Kneidinger *et al.*, Physica C: Superconductivity and its Applications **514**, 388 (2015)
M. Smidman *et al.*, Reports on Progress in Physics **80**, 036501 (2017)
S. Yip, Annual Review of Condensed Matter Physics **5**, 15 (2014)

Question to address

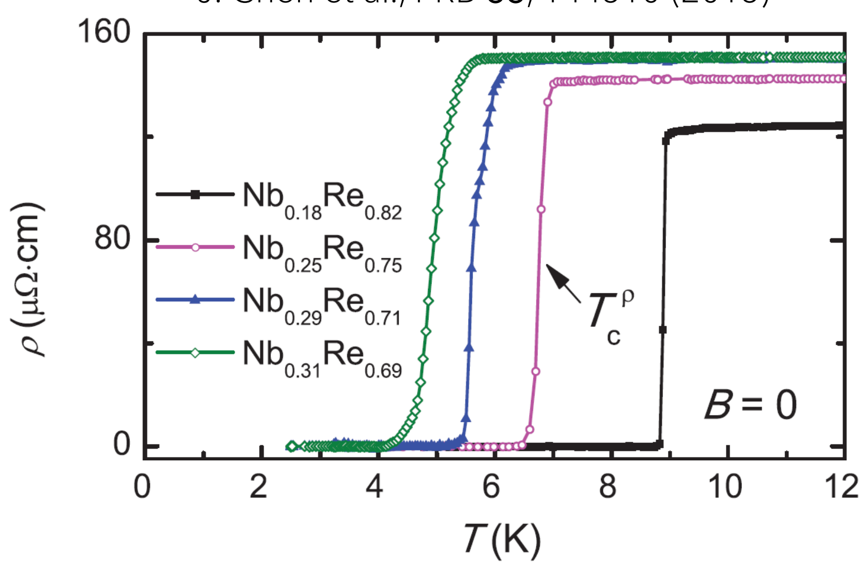
Can a weakly-correlated and phonon-driven NCS host mixed-parity superconductivity?

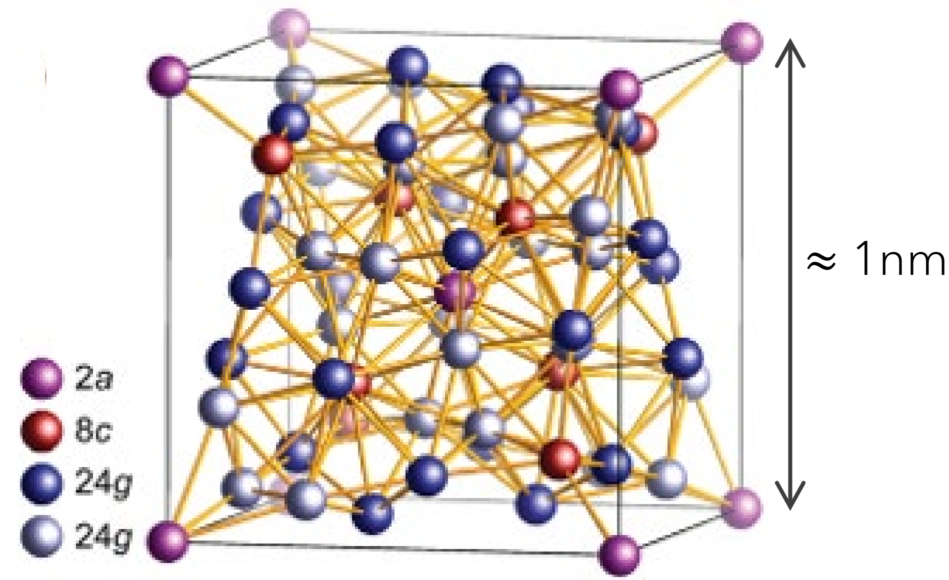
Can STM/STS studies contribute to resolving the order parameter symmetry?

Noncentrosymmetric compound Nb-Re

- Nb_xRe_{1-x} ($0.13 \leq x \leq 0.38$): strongly composition-dependent critical temperature T_c
- Highest sample quality and T_c for the $x = 0.18$ stoichiometry ($Nb_{0.18}Re_{0.82}$)

J. Chen et al., PRB **88**, 144510 (2013)





Unit cell of the body-centered cubic α-Mn crystal structure ($a \approx 9.6$ Å for $x = 0.18$)

K. Stolze et al., J. Mater. Chem. C **6**, 10441 (2018)

Nb-Re: A still-puzzling superconductor

Evidence for **s-wave superconductivity** in non-centrosymmetric $Re_{24}Nb_5$ from ^{93}Nb NMR measurements
Lue *et al.*, PRB **84**, 052509 (2011)

BCS-like superconductivity in the non-centrosymmetric compounds Nb_xRe_{1-x} ($0.13 \leq x \leq 0.38$)
Chen *et al.*, PRB **88**, 144510 (2013)

Time-Reversal Symmetry Breaking in Re-Based Superconductors
Shang *et al.*, PRL **121**, 257002 (2018)

Unveiling **Intrinsic Triplet Superconductivity** in Noncentrosymmetric NbRe through Inverse Spin-Valve Effects
Colangelo *et al.*, PRL**135**, 226002 (2025)

?

State of research

Literature reports on both **conventional and unconventional** superconductivity (mostly on disordered thin films)

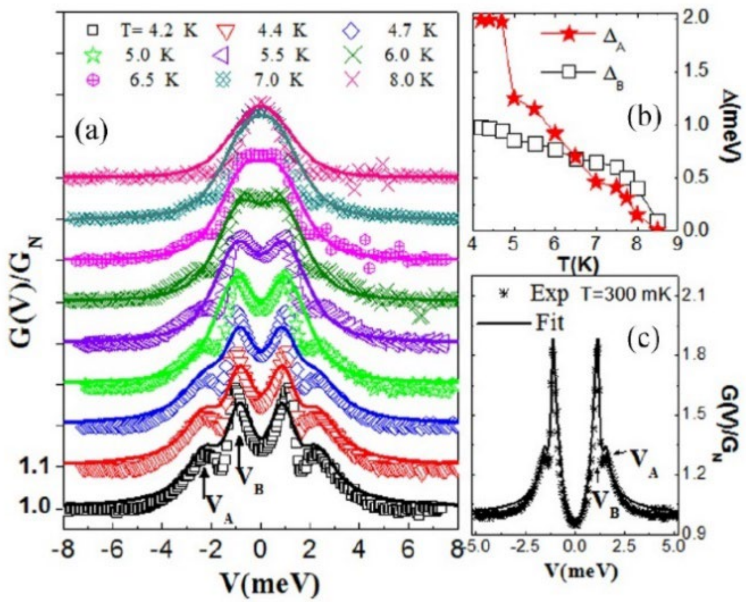
Weakly correlated material

- Wilson ratio $R_W = 0.94$
- Kadowaki-Woods ratio (KWR)

$$A/\gamma^2 = 0.24 \times 10^{-5}\,\mu\Omega\mathrm{cm}/(\mathrm{mJ/mol\,K})^2$$

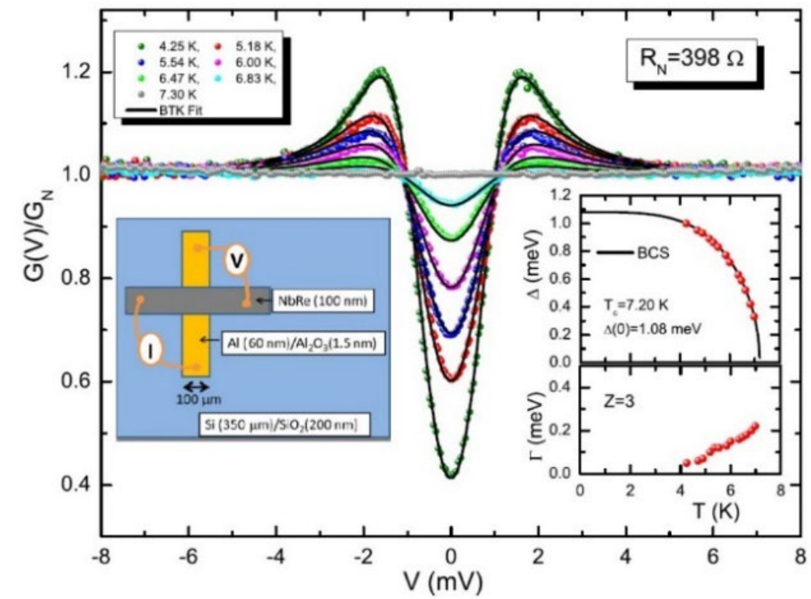
Controversial reports on the superconducting OP

Point-contact spectroscopy on single crystals
Two-gap model of isotropic s-wave pairing



C. Cirillo et al., PRB **91**, 134508 (2015)

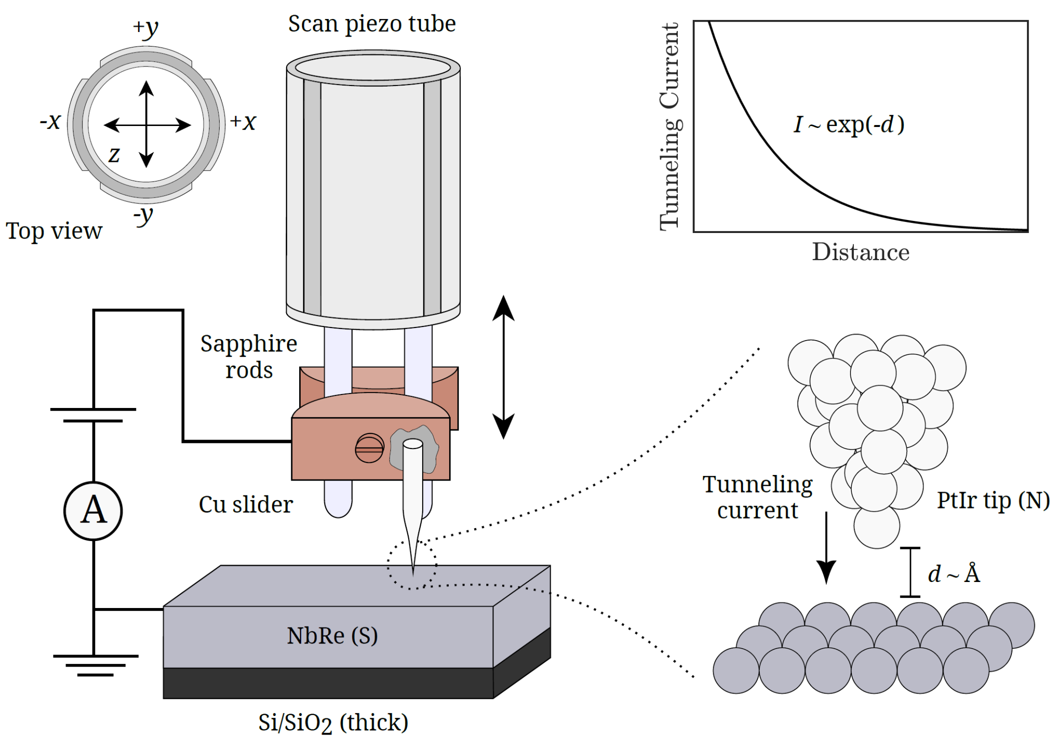
Thin film tunnel junctions (N-I-S junction)
Single-gap model of isotropic s-wave pairing



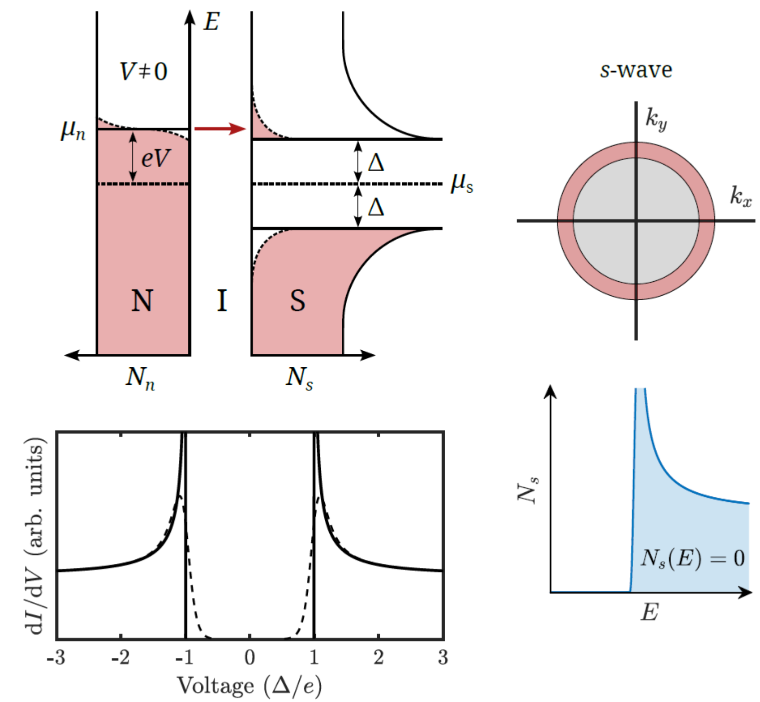
C. Cirillo et al., PRB **94**, 104512 (2016)

Spatially-resolved transport measurements!

Probing the local density of states (DOS) by STM

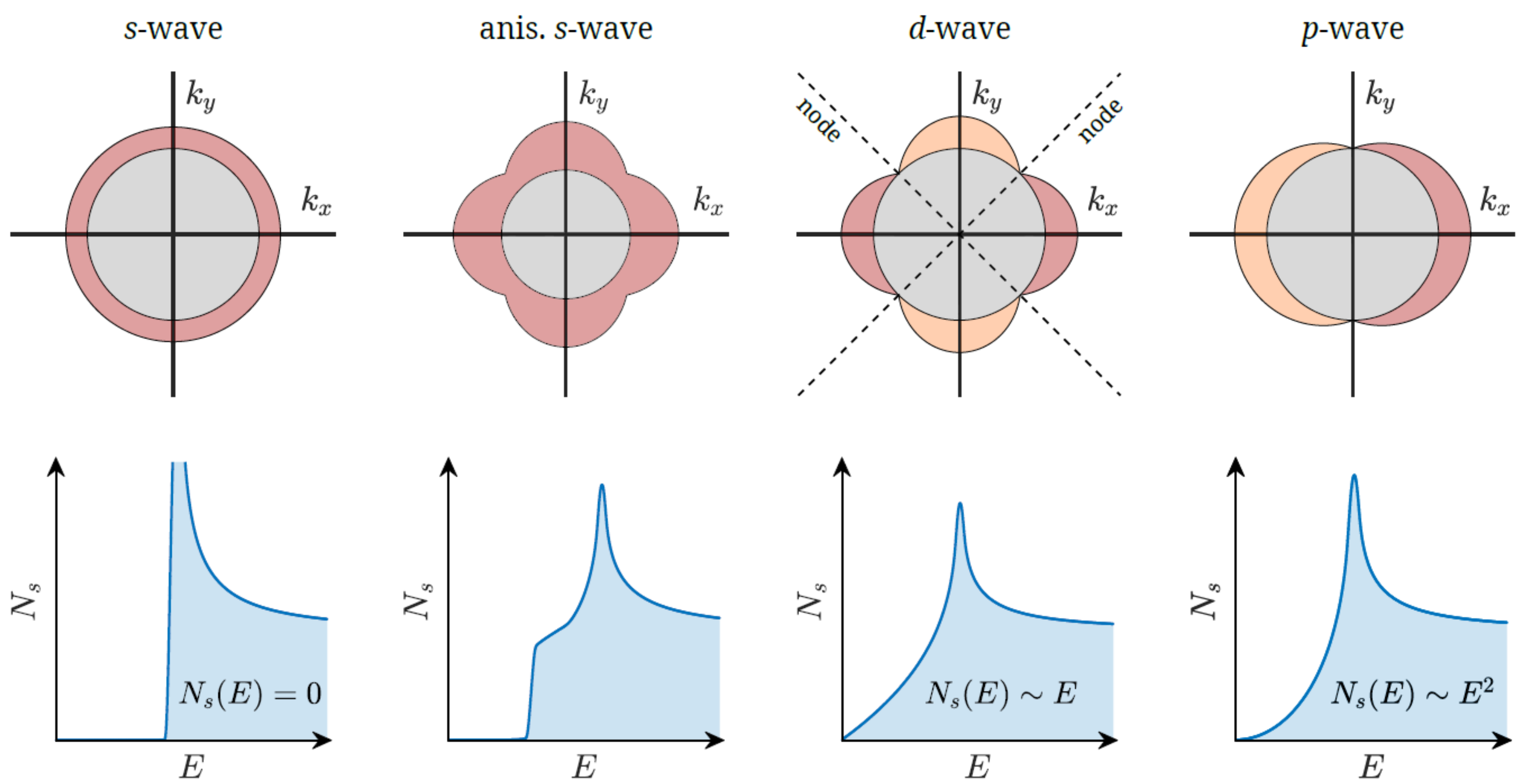


T = 300mK



$$\frac{\mathrm{d}I}{\mathrm{d}V}(V) \propto \int_{-\infty}^{\infty} \mathrm{d}E' \, N_s(E') \left(-\frac{\partial f(E' - eV, T)}{\partial E'} \right)$$

Orbital order-parameter symmetries

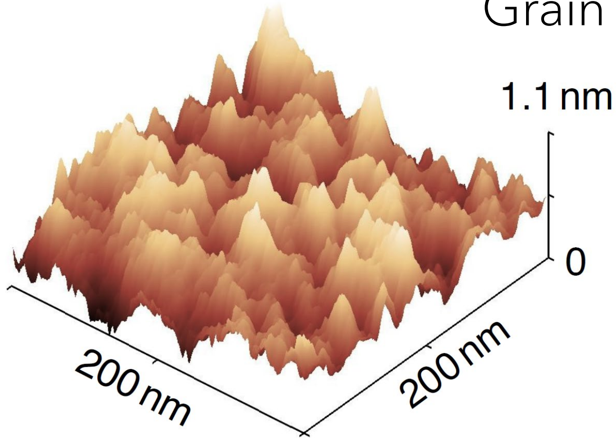


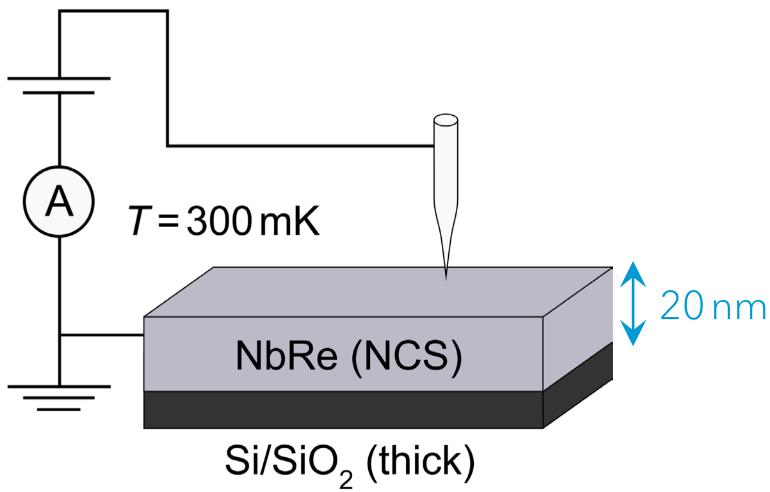
k-space symmetry

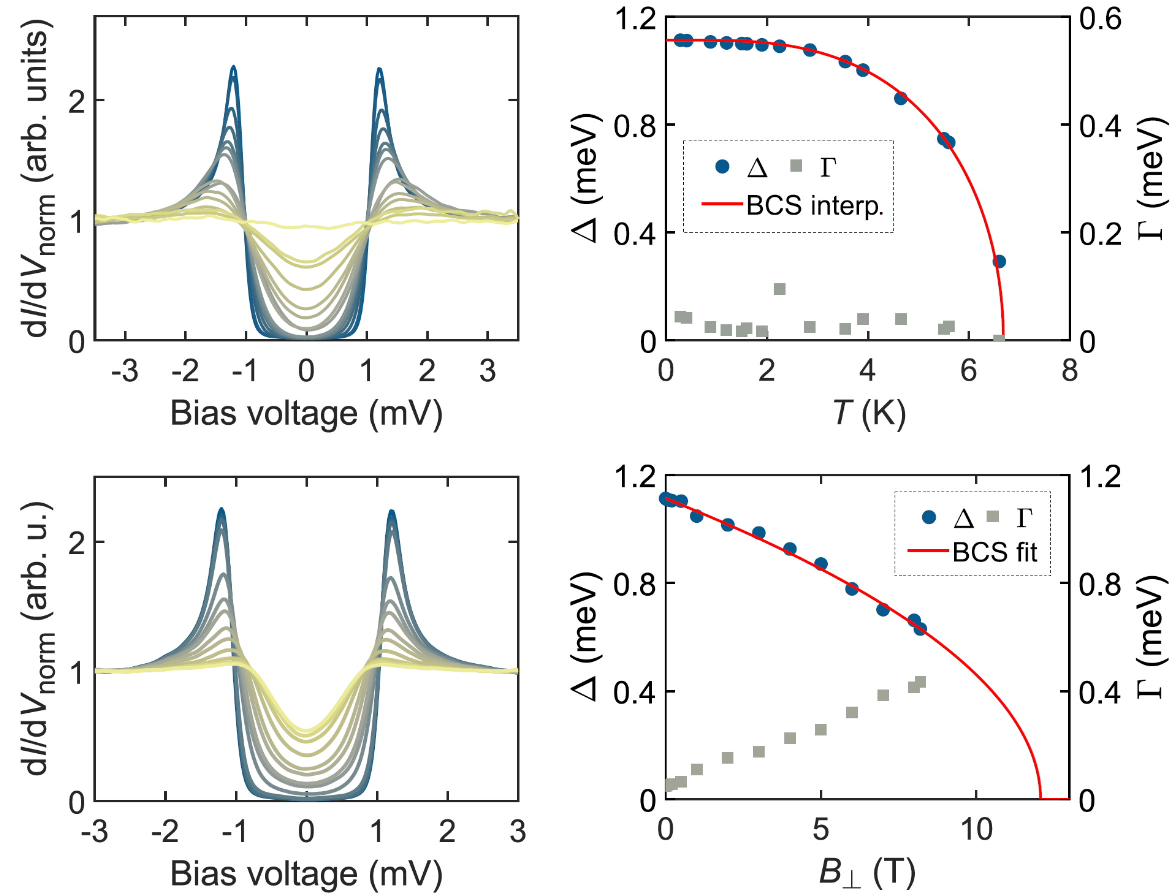
DOS „fingerprint"

Spectroscopic evidence for nodal SC in Nb-Re thin films

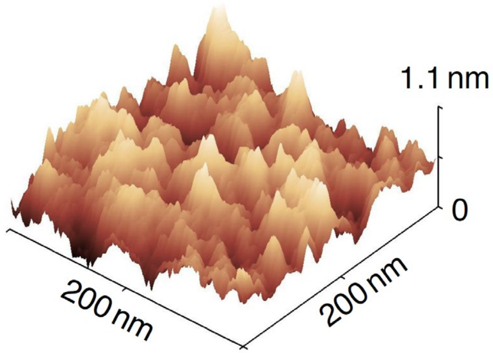
Grain size ~ 5-10 nm



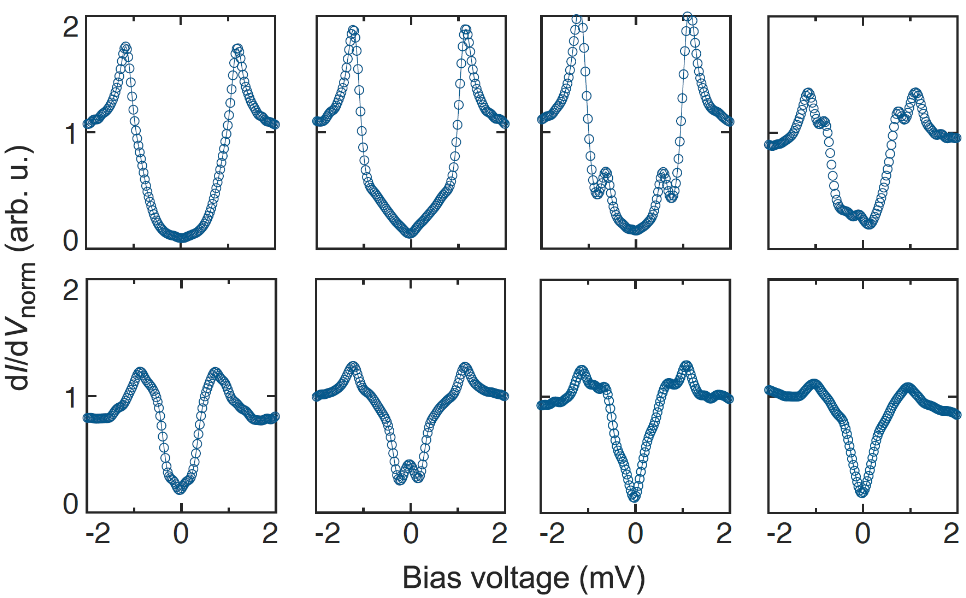


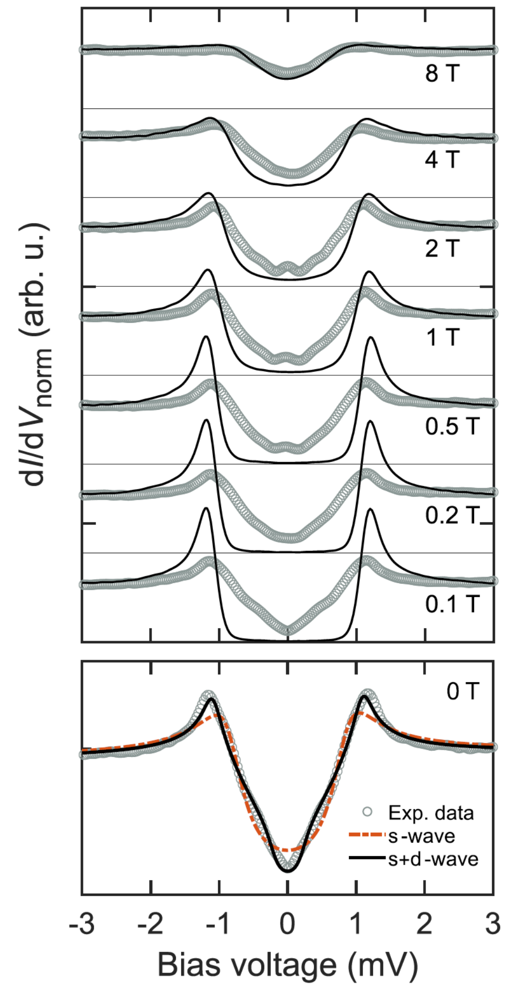


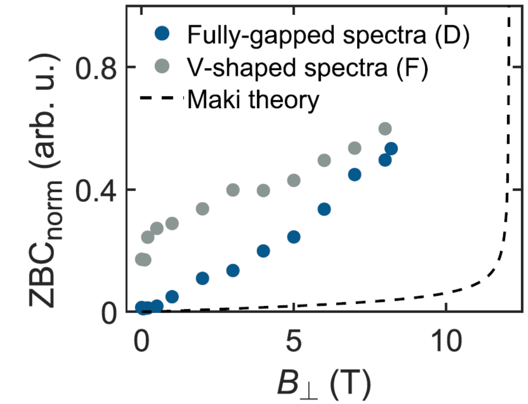
Spectroscopic evidence for nodal SC in Nb-Re thin films

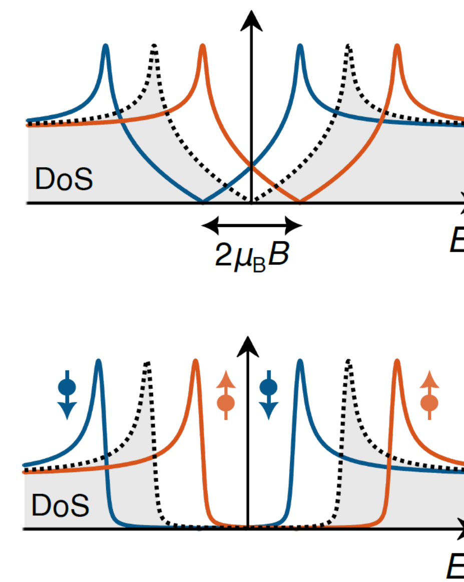


Spatial variations of the LDOS

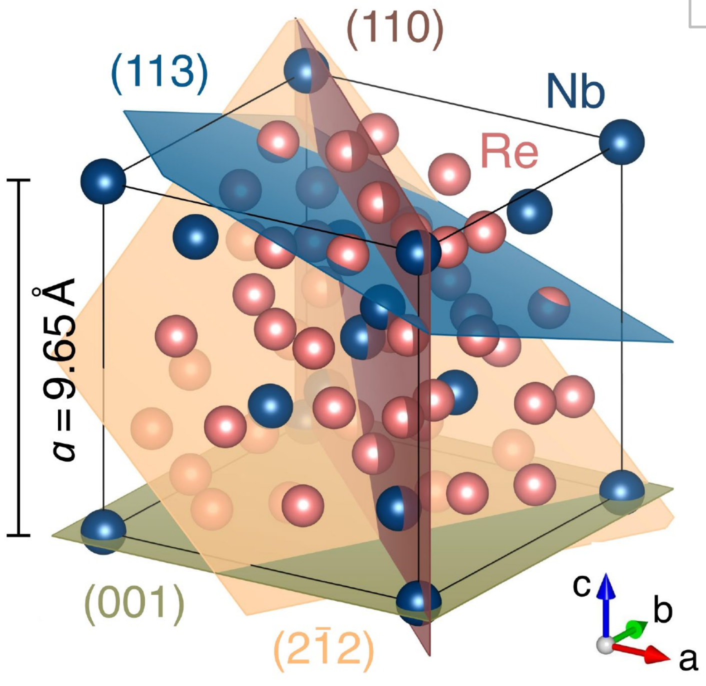






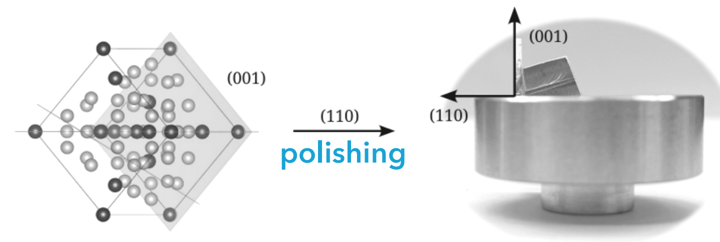


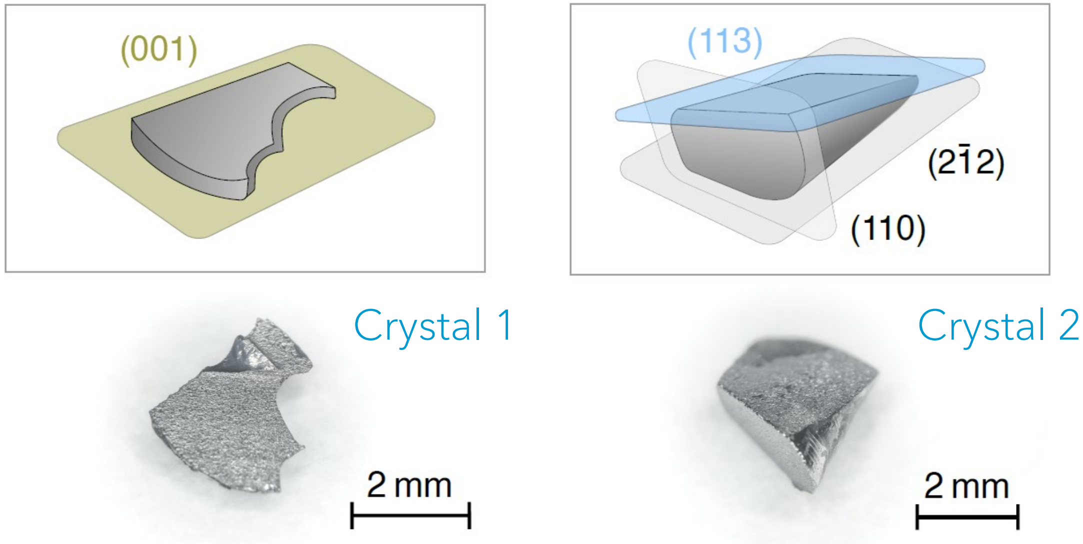
Orientation-dependent tunneling in Nb-Re single crystals



Surface treatment

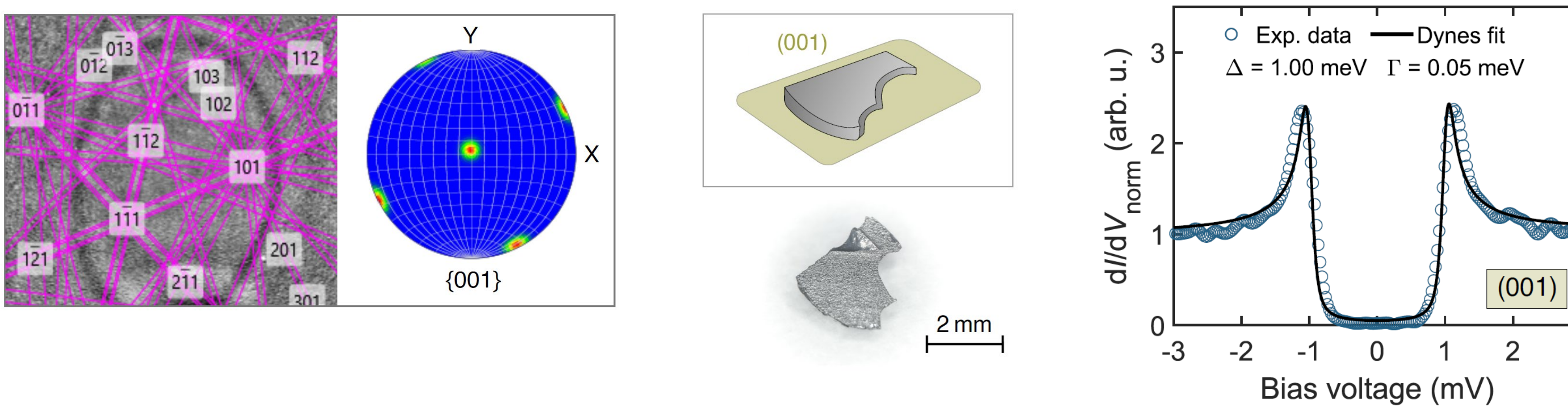
- Diamond Polishing
- Ar Milling
- EBSD/XRD

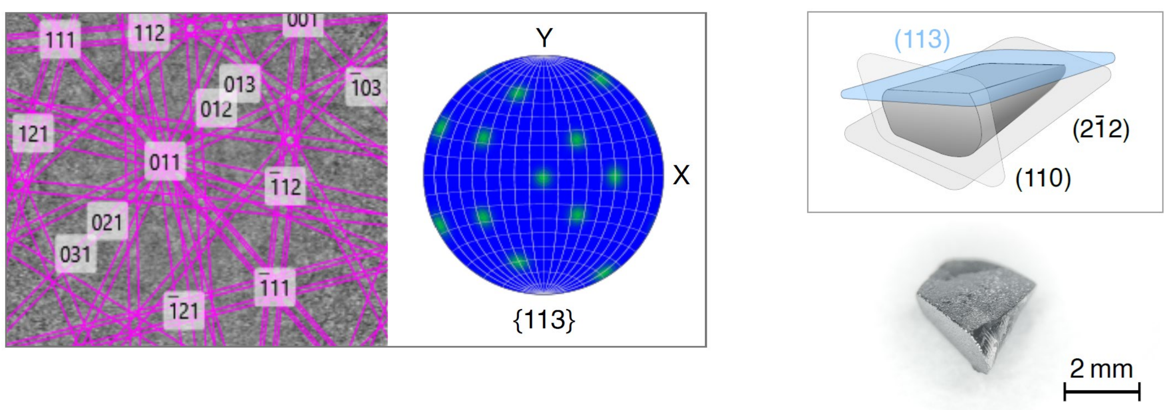


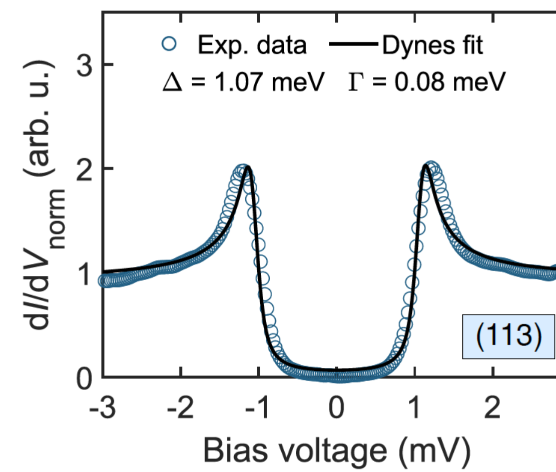


Thanks to M. Smidman & G. Balakrishnan (Univ. Warwick)

Orientation-dependent tunneling in Nb-Re single crystals



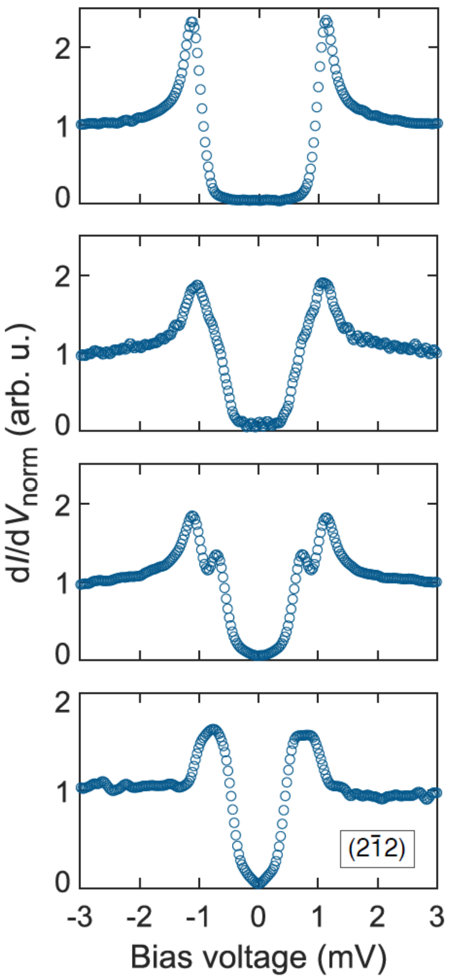




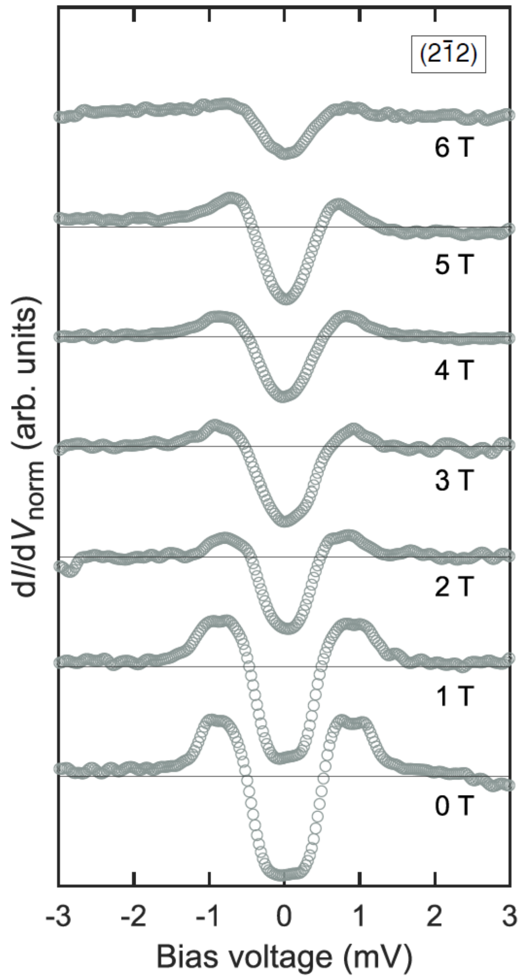
BCS-type spectra on (001) and (113) surface

Orientation-dependent tunneling into $(2\bar{1}2)$ plane

Spatial variations

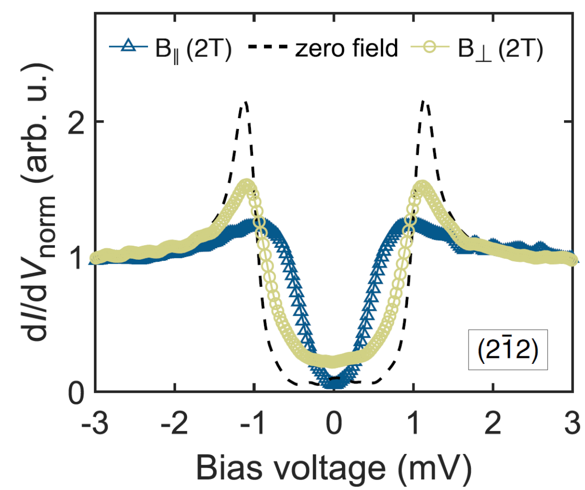


B-field dependence



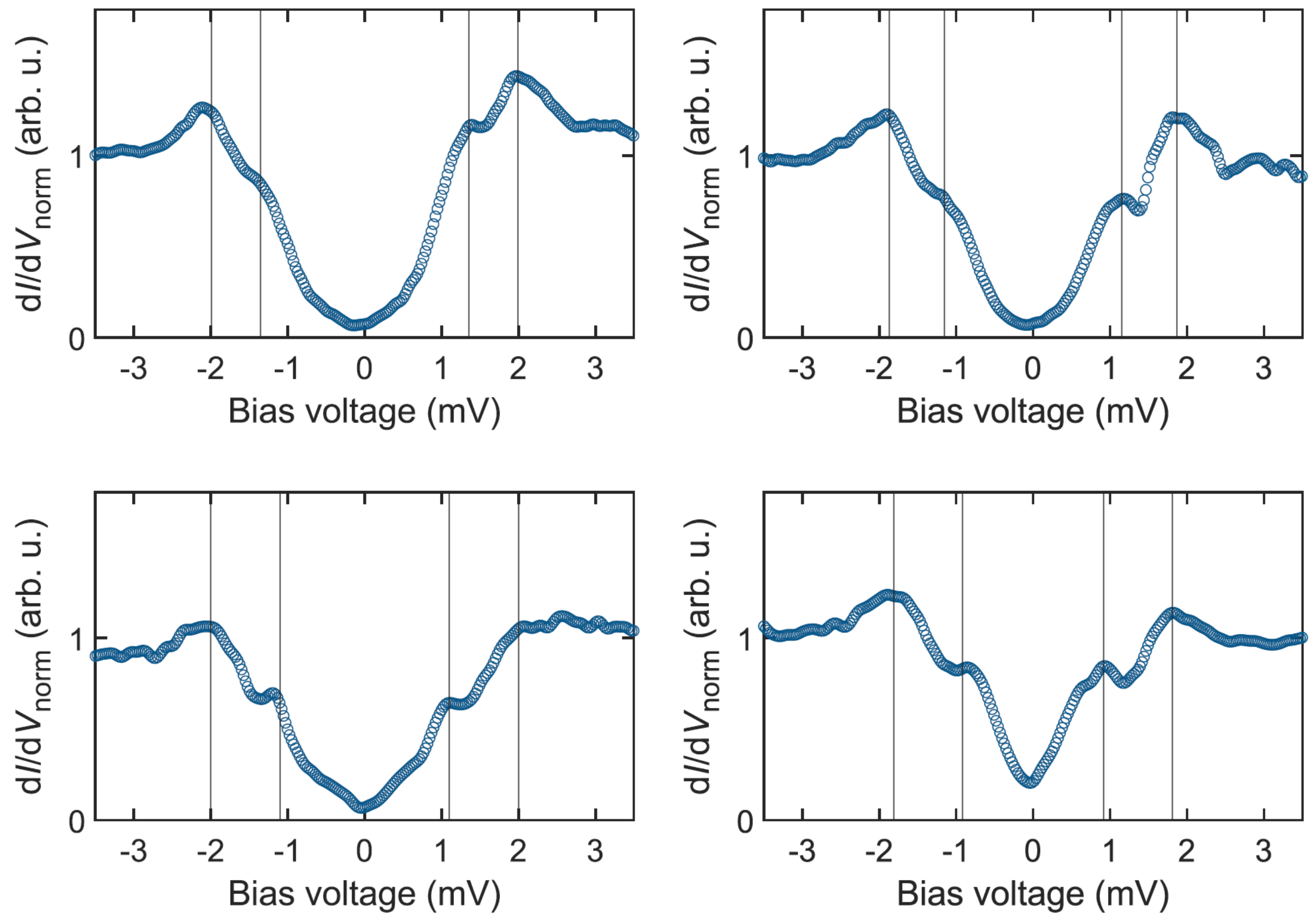
- Fully-gapped and V-shaped tunnel spectra
- Prominent in-gap signatures
- Highly-anisotropic gap suppression in magnetic fields

Consistent with an anisotropic two-component order parameter



Orientation-dependent tunneling into (110) plane

Enlarged gap with Δ ~ 2 meV



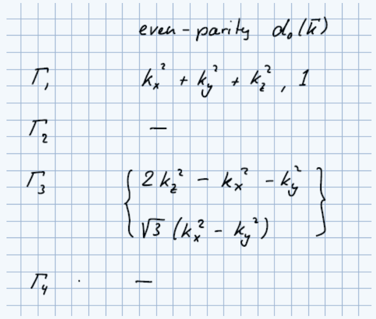
Unveiling the superconducting order parameter

Symmetry-constrained theory

Space group
Point group

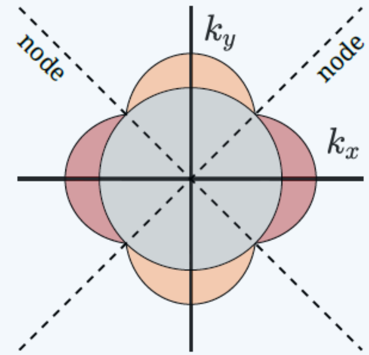
Antisymmetric spin-orbit coupling (ASOC)

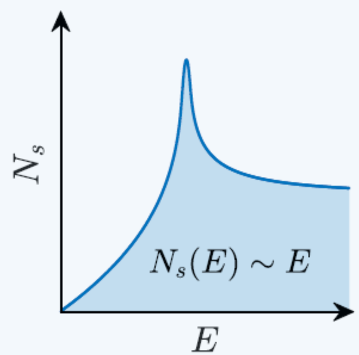
Odd-/even gap functions



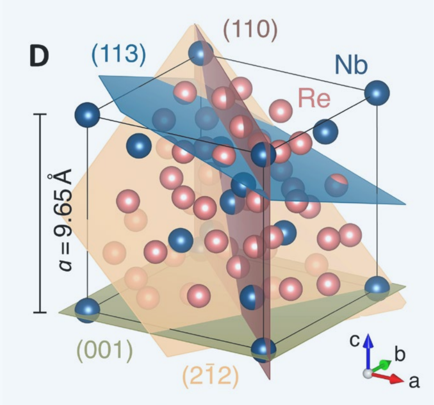
Thanks to M. Sigrist (ETH Zurich)

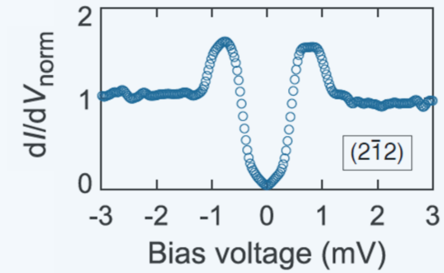
Anisotropic 3D OP, DOS





Multidirectional tunneling





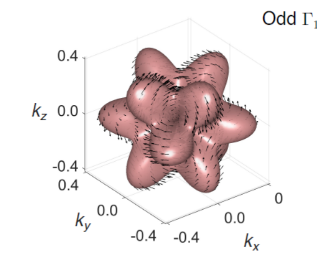
Even- and odd-parity basis functions

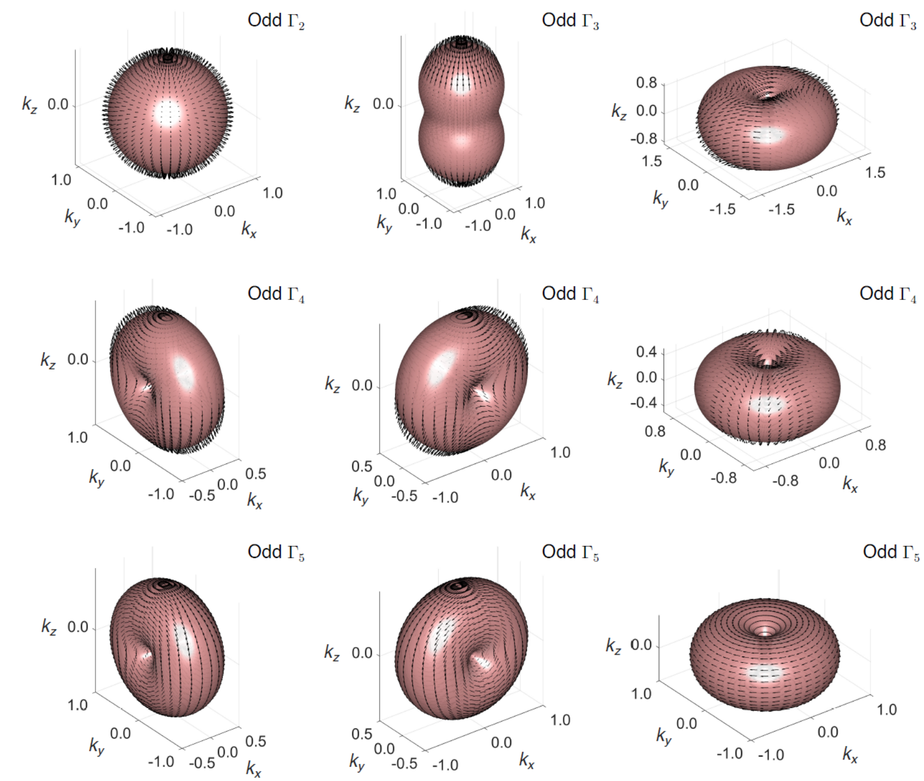
	even parity $\psi(\mathbf{k})$	**odd** parity $\mathbf{d}(\mathbf{k})$
Γ_1	$k_x^2+k_y^2+k_z^2,\ 1$	$\hat{x}k_x(k_y^2-k_z^2)+\hat{y}k_y(k_z^2-k_x^2)+\hat{z}k_z(k_x^2-k_y^2)$
Γ_2	–	$\hat{x}k_x+\hat{y}k_y+\hat{z}k_z$
Γ_3	$\{2k_z^2-k_x^2-k_y^2,\ \sqrt{3}(k_x^2-k_y^2)\}$	$\{2\hat{z}k_z-\hat{x}k_x-\hat{y}k_y,\ \sqrt{3}(\hat{x}k_x-\hat{y}k_y)\}$
Γ_4	–	$\{\hat{y}k_z+\hat{z}k_y,\ \hat{z}k_x+\hat{x}k_z,\ \hat{x}k_y+\hat{y}k_x\}$
Γ_5	$\{k_yk_z,\ k_zk_x,\ k_xk_y\}$	$\{\hat{y}k_z-\hat{z}k_y,\ \hat{z}k_x-\hat{x}k_z,\ \hat{x}k_y-\hat{y}k_x\}$

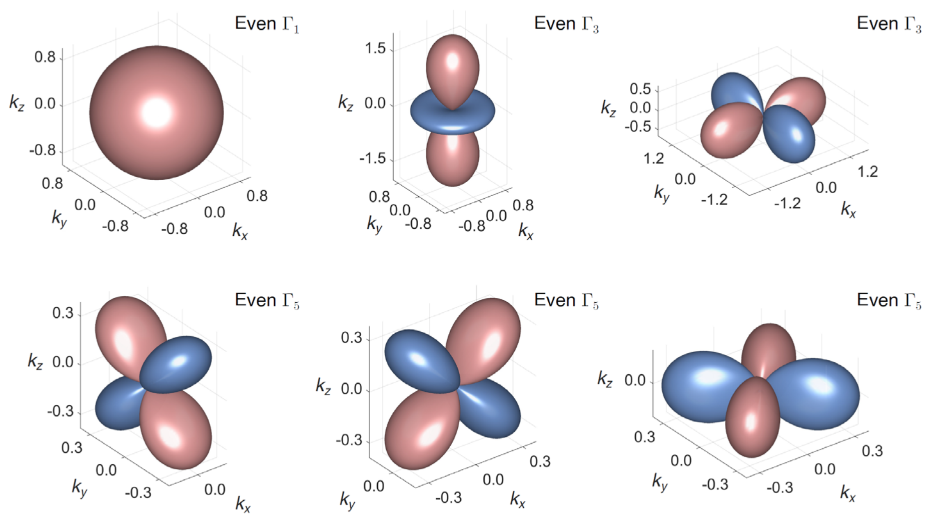
Antisymmetric SOC: $\gamma_{\mathbf{k}}=\left(k_x(k_y^2-k_z^2),k_y(k_z^2-k_x^2),k_z(k_x^2-k_y^2)\right)$

Space group: I-43m

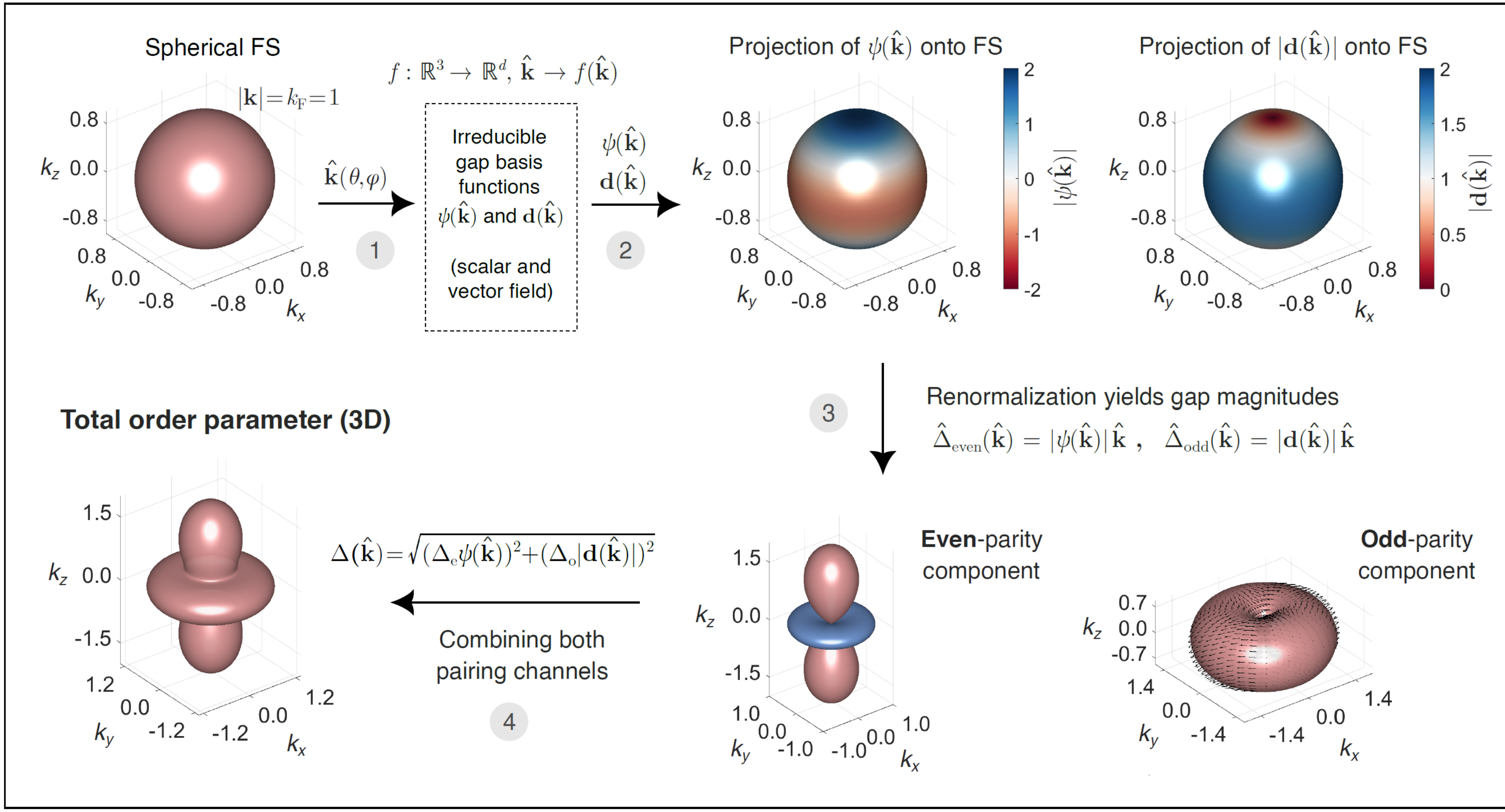
Point group: T_d





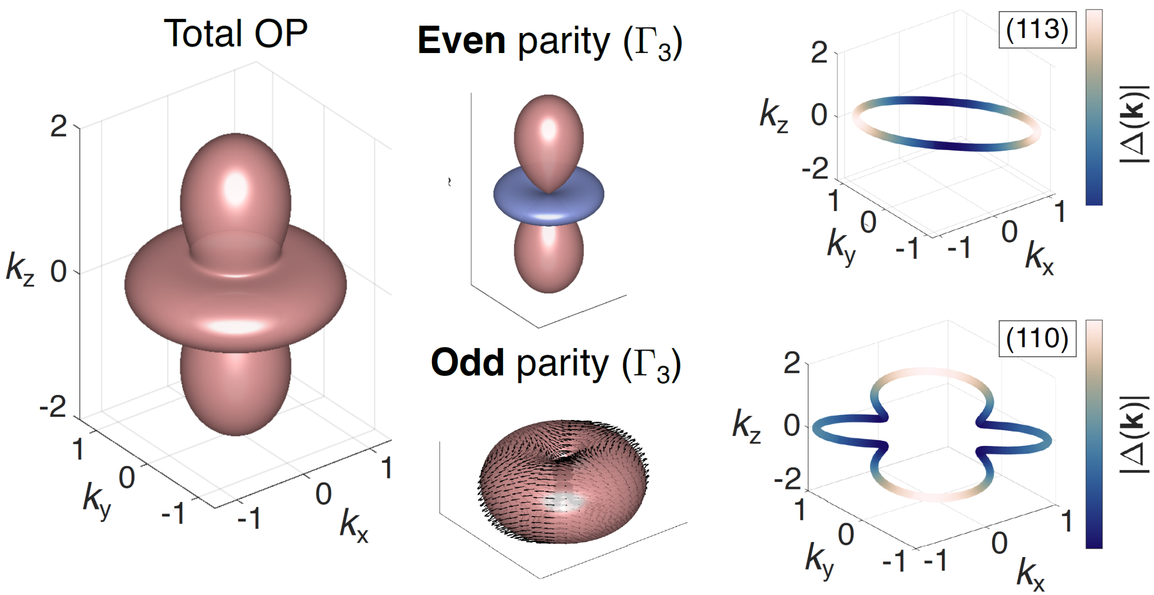


Calculation of the total mixed-parity order parameter



Tunneling model (preliminary)

Cross-sectional **2D line profiles** in k-space (orientation dependent!)



In-plane tunneling

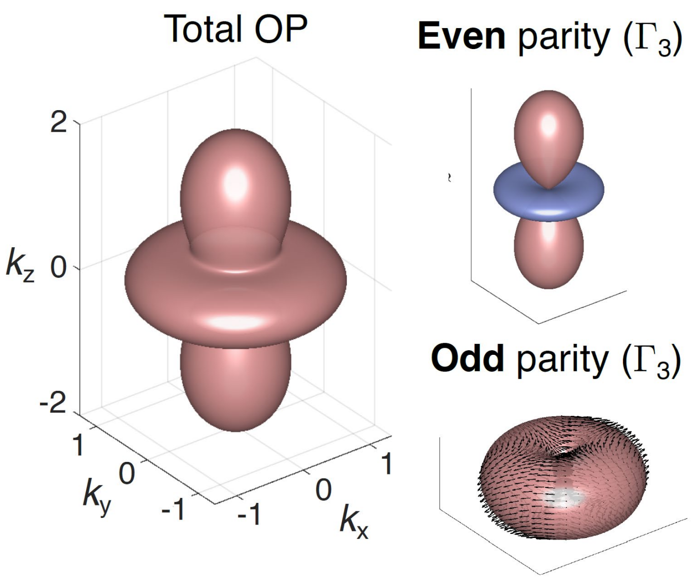
Considering predominantly in-plane momenta $k_{\|}$ renders the quasiparticle DoS

$$N_s(E) = \left\langle \mathrm{Re}\left[\frac{|E|}{\sqrt{E^2 - |\Delta(\mathbf{k})|^2}}\right]\right\rangle_{\mathbf{k}_{\|},\,\mathrm{FS}}$$

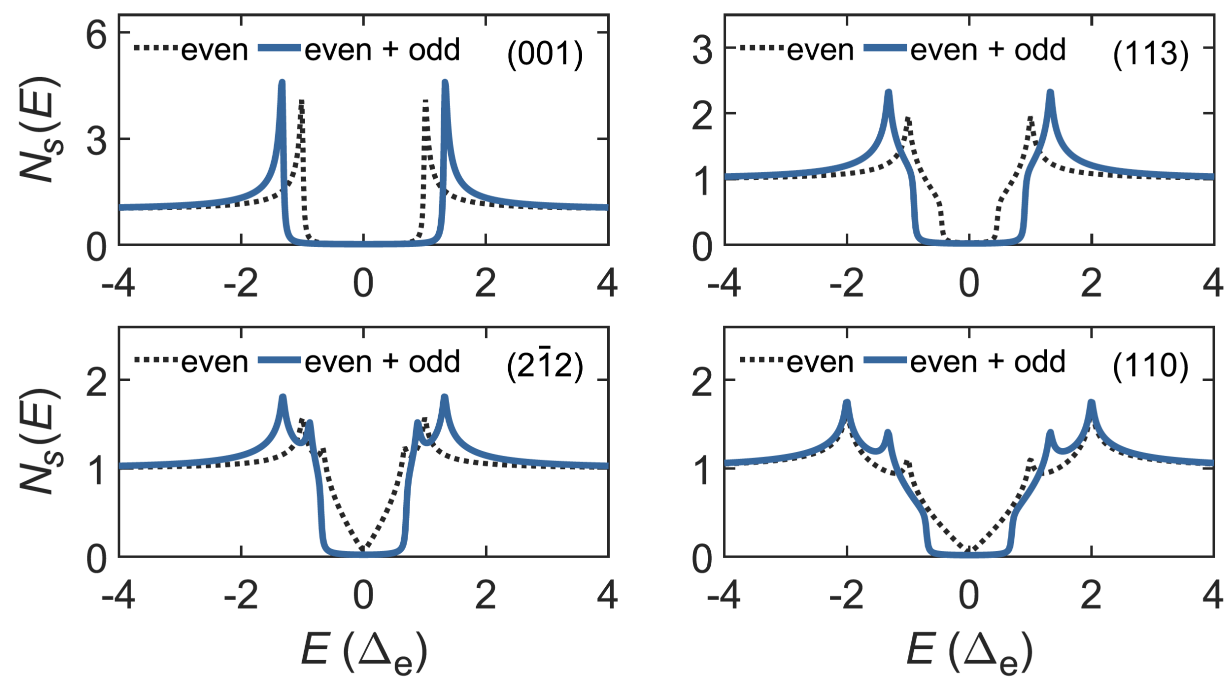
highly orientation dependent

Tunneling model (preliminary)

Mixed-parity OP with (**d_{z^2} + toroidal**) –orbital shape reproduces the whole spectroscopic dataset



Orientation-dependent modeling



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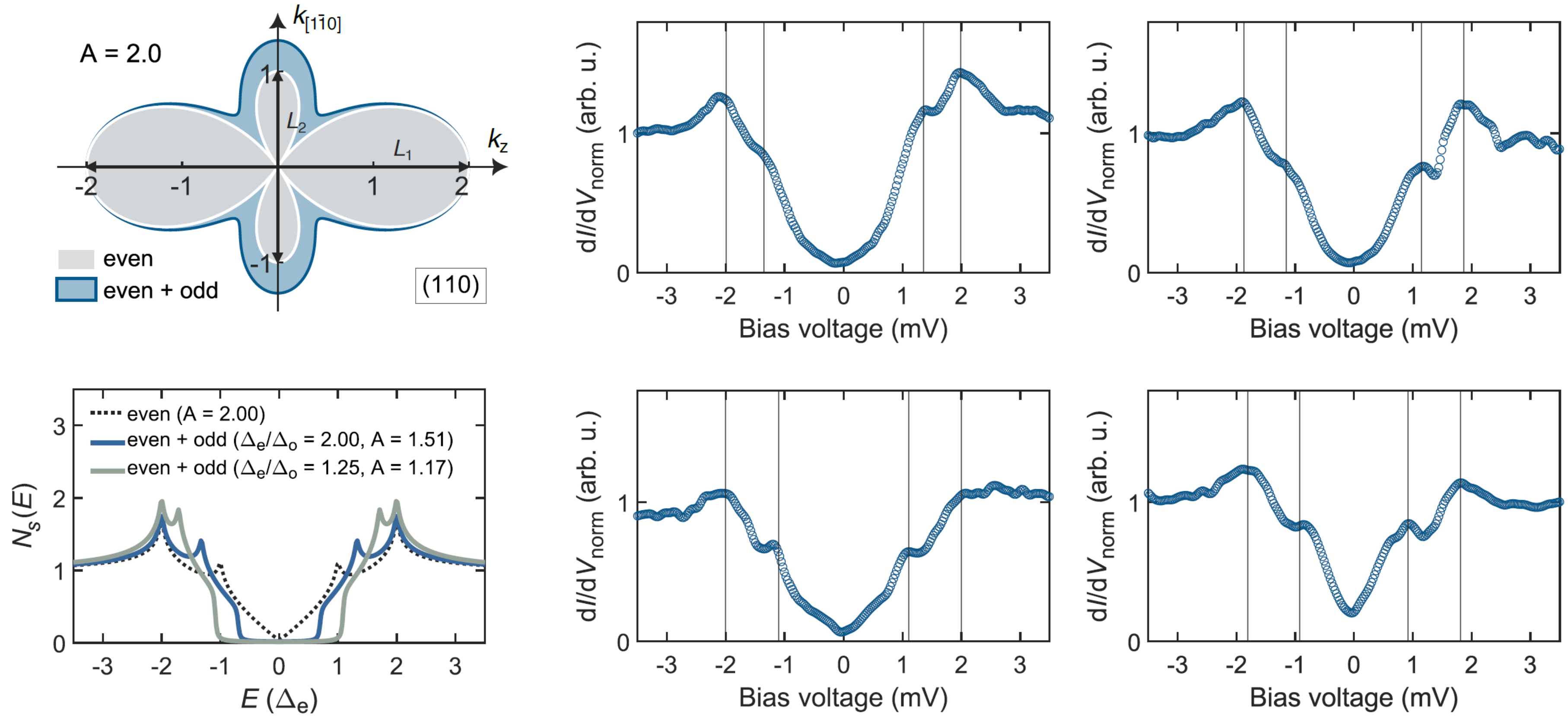
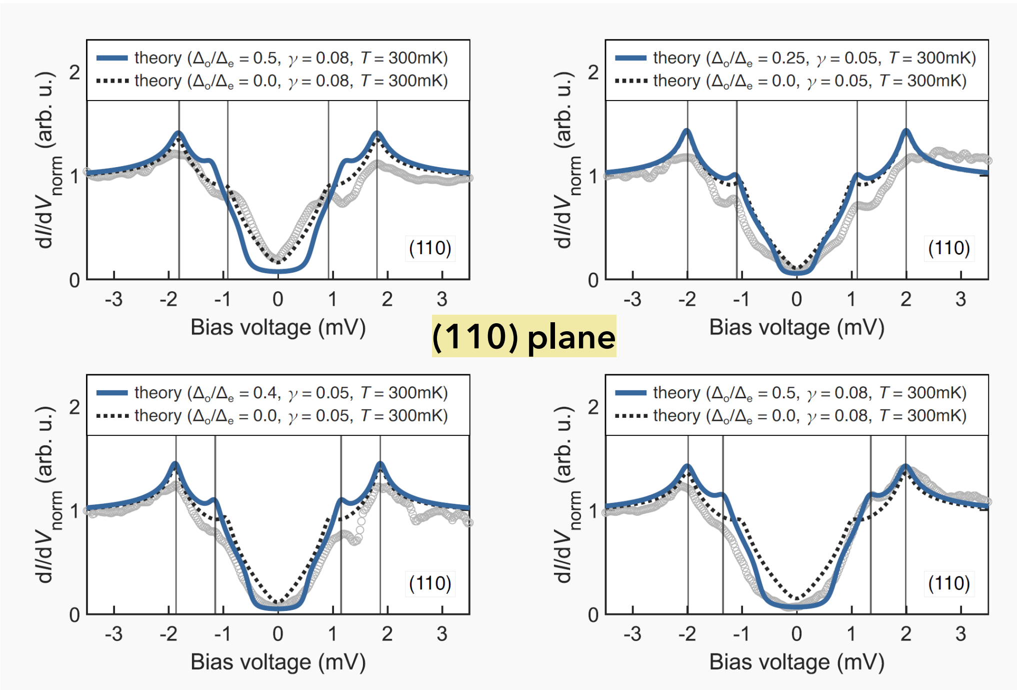
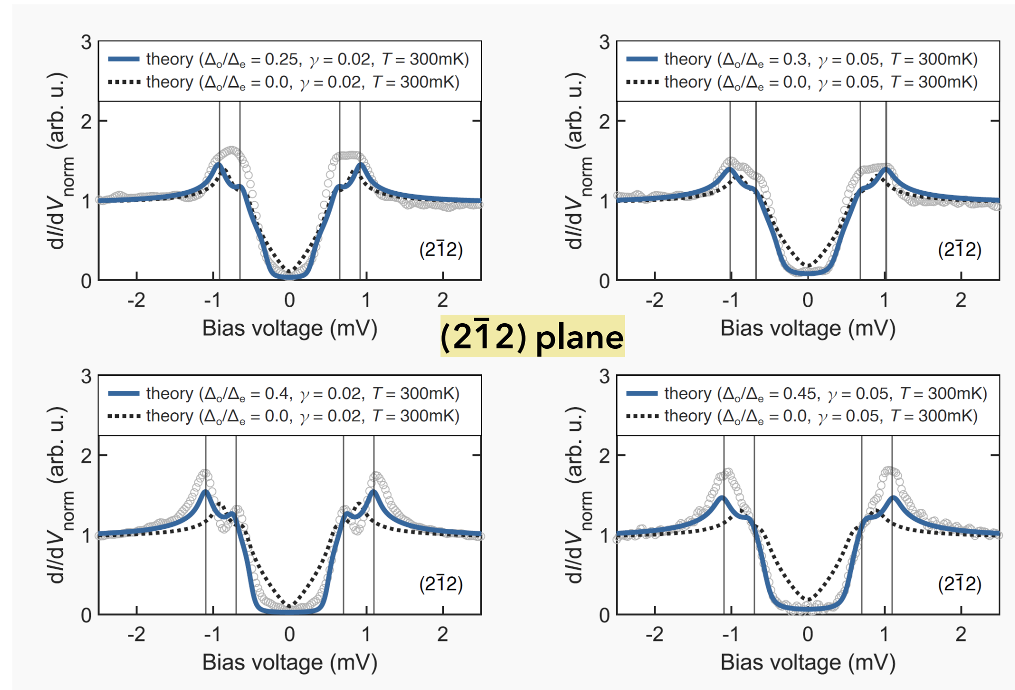


Estimation of the spin-triplet amplitude

Mixed-parity OP with (**d_z^2 + toroidal**) –orbital shape: $|\Delta(\mathbf{k})| = \sqrt{(\Delta_e|\psi(\mathbf{k})|)^2 + (\Delta_o|\mathbf{d}(\mathbf{k})|)^2}$



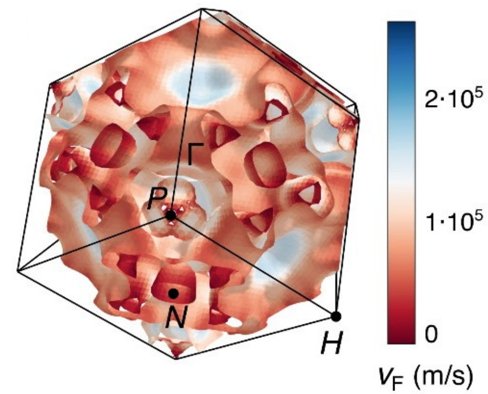


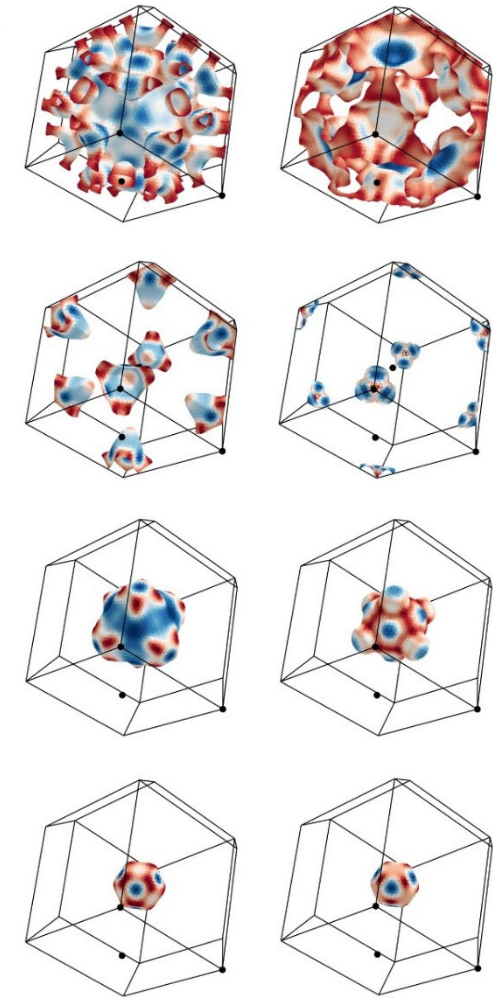
$\Longrightarrow$ Triplet-to-singlet ratio Δ_o/Δ_e reaches up to ~40%

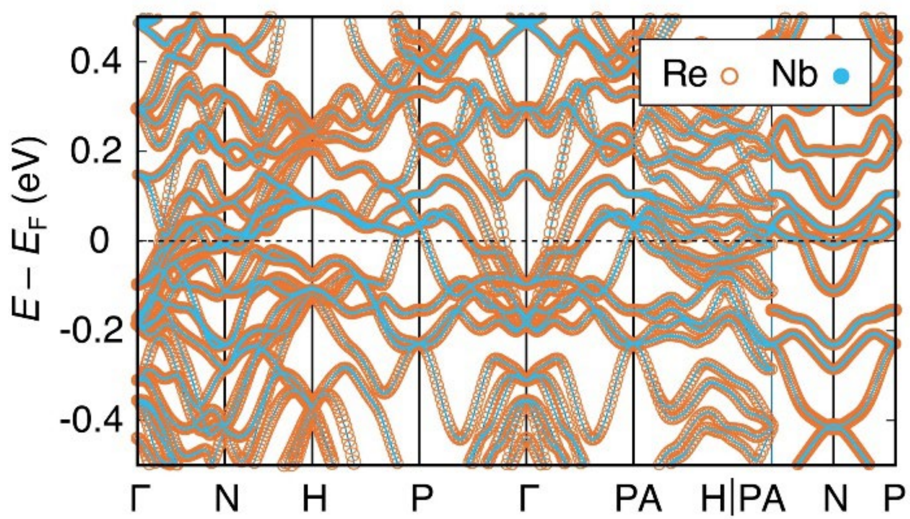
Can an anisotropic, two-component OP be expected?

Band-structure calculations reveal

- Eight bands cross the Fermi surface
- Fermi velocity $v_F \sim 1.5 \times 10^5\,\frac{\mathrm{m}}{\mathrm{s}}$
- Band splitting $E_{\mathrm{ASOC}} \sim 100\ \mathrm{meV}$







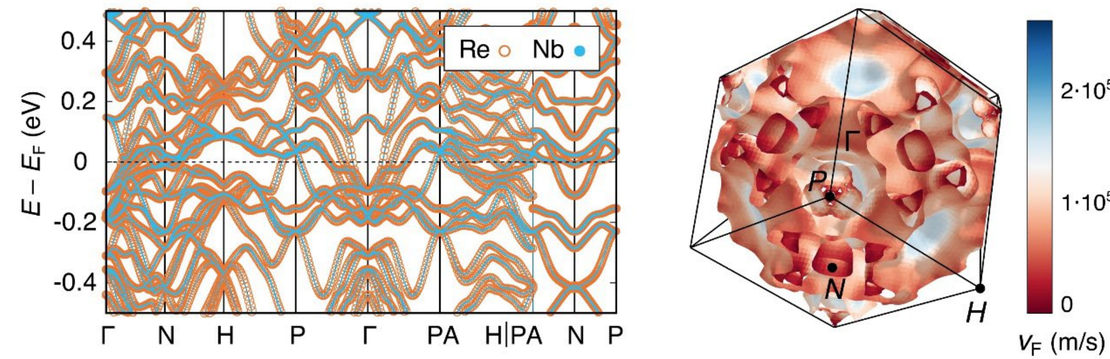
Vienna **A**b initio **S**imulation **P**ackage (Vasp)

Thanks to A. Smolyanyuk and K. Held (TU Wien)

Can an anisotropic, two-component OP be expected?

Band-structure calculations reveal

- Eight bands cross the Fermi surface
- Fermi velocity $v_F \sim 1.5 \times 10^5 \, \frac{\mathrm{m}}{\mathrm{s}}$
- Band splitting $E_{\mathrm{ASOC}} \sim 100 \text{ meV}$



Thanks to A. Smolyanyuk & K. Held (TU Wien)

Estimation of the clean-limit superconducting coherence length (= upper bound)

$$\xi \approx \frac{\hbar v_F}{\pi \Delta} \approx 30 \text{ nm}$$

Band-splitting energy E_{ASOC} as an indicator for spin-triplet contribution

$$E_r = \frac{E_{\mathrm{ASOC}}}{k_B T_c} \approx 130$$

NCS compounds	E_{ASOC} (meV)	E_r	Pairing state
$CePt_3Si$	200	3093	$s+p$
Li_2Pt_3B	200	892	triplet
BiPd	50	157	two-gap
$LaNiC_2$	42	177	two-gap
Y_2C_3	15	11	two-gap
Li_2Pd_3B	30	46	s-wave
La_2C_3	30	26	s-wave

Replotted from: Jiao *et al.*, Phys. Rev. B **89**, 060507 (2014)

Tunneling model – Open questions

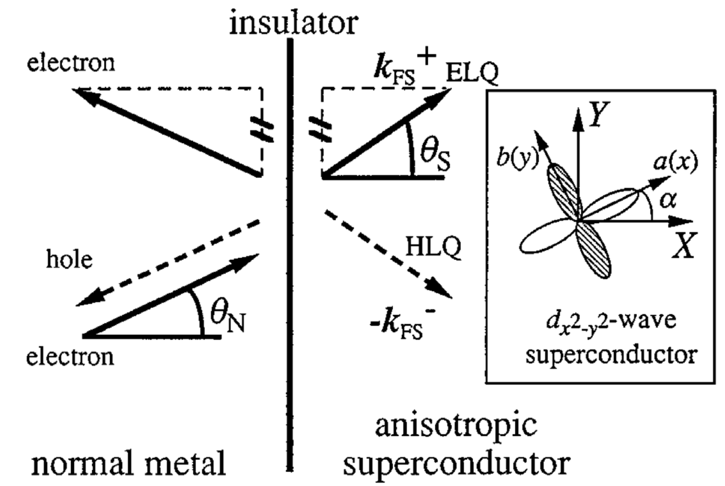
What make surface-parallel momenta dominating?

- Tunneling spectra of anisotropic superconductors

  Kashiwaya and Tanaka *et al.*, PRB **52**, 2667 (1998)

  Conservation of k along the planar interface:

  $$k_{\mathrm{FS}}\sin\theta_S = k_{\mathrm{FN}}\sin\theta_N$$



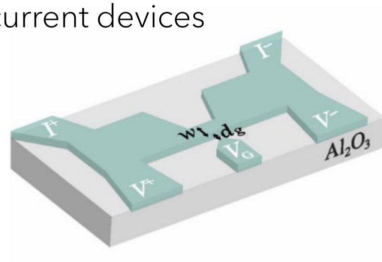
- Role of bulk vs (topological) surface states?

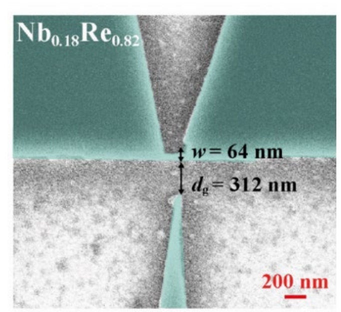
- Particularity of tunneling into NCS

  arXiv:1001.2486 [cond-mat.supr-con] M. Eschrig, C. Iniotakis, Y. Tanaka: Theoretical aspects of Andreev spectroscopy and tunneling spectroscopy in non-centrosymmetric superconductors: a topical review

- **Summary:**
  - Parity-mixed NCS = Platform to study formation of spin-triplet pairing (w/o strong correlations)
  - Multiple OP signatures in Nb-Re thin films
  - Orientation-dependent tunneling in single crystals
  - Modeling suggests nodal mixed-parity OP
- **Conclusion:** Substantial parity mixing in a weakly-correlated, phonon-driven NCS with strong ASOC
- **Outlook:** Application in superspintronic devices

J. Koch et al., Nano Res. **17**, 6575 (2024)
Gate-controlled supercurrent devices
(Univ. Konstanz)





Universität
Konstanz

Nodal superconductivity with spin-triplet component in a noncentrosymmetric weakly-correlated metal

arXiv:2606.04742 [cond-mat.supr-con]

arXiv:
2606.04742

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Thank you for your attention!

Universität Konstanz

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