Evidence of strong correlations and unconventional superconductivity in monolayer transition metal dichalcogenides 1H-$NbSe_2$ and 1H-TaS_2

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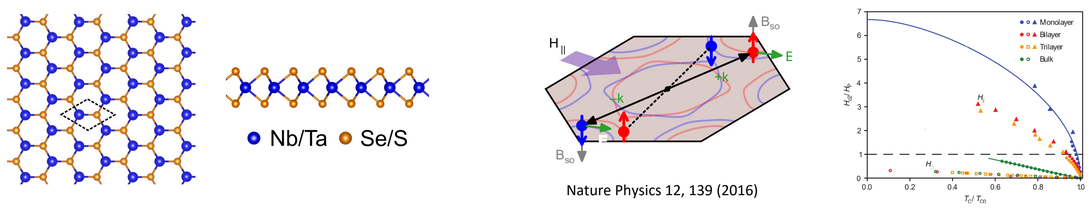
1H-$NbSe_2$ and 1H-TaS_2: Monolayer Ising superconductors



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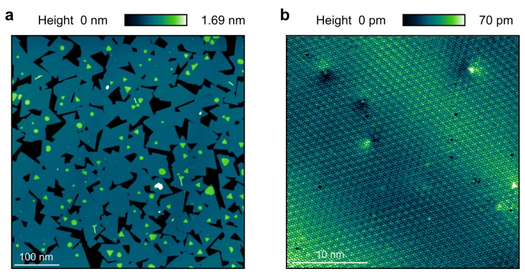
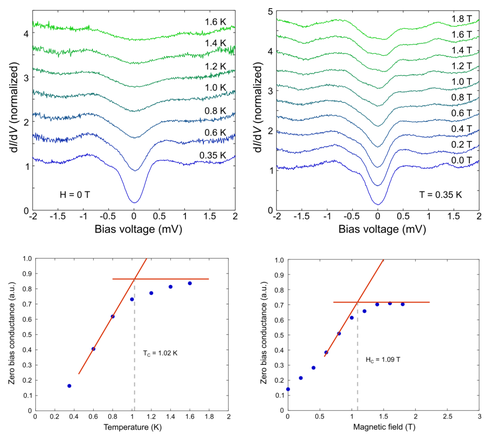
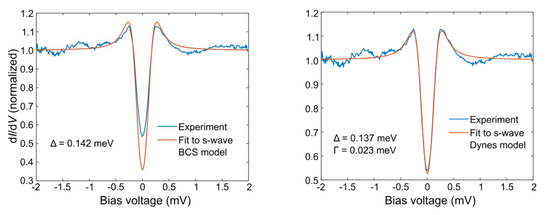
- Broken inversion symmetry leads to in-plane crystal field **E.** Spin-orbit coupling $\mathbf{B_{so}} \propto \mathbf{E} \times \mathbf{k}$ is out-of-plane: spins are locked
- Pauli paramagnetic limit is surpassed for applied in-plane field

1H-TaS_2/HOPG



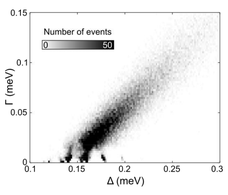


Fitting the superconducting spectra



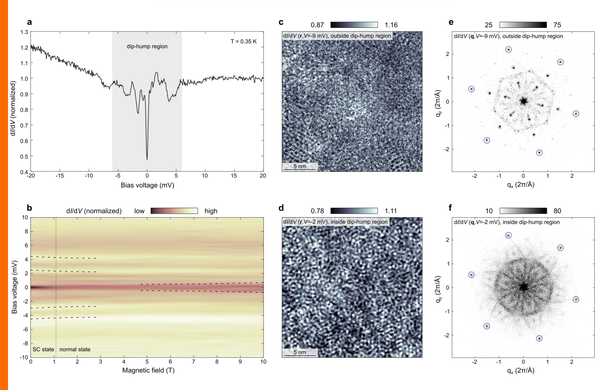
s-wave BCS model: $\rho(E) = \left|\Re\left[\frac{E}{\sqrt{E^2-\Delta^2}}\right]\right|$

s-wave Dynes model: $\rho(E) = \left|\Re\left[\frac{E-i\Gamma}{\sqrt{(E-i\Gamma)^2-\Delta^2}}\right]\right|$



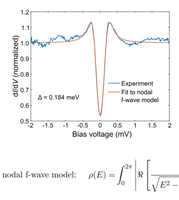
Δ and Γ should not be correlated!

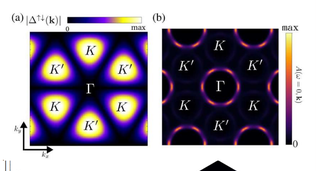
Presence of many body excitations



Pairing symmetry

- L = 0 (s-wave) inconsistent
- $s^{\pm}$ stems from inter-band repulsive interactions in a multiband electronic structure ⇨inconsistent
- L = 1 ⇨ Either fully gapped p+ip or nodal nematic ⇨ inconsistent
- L = 2 ⇨ Either fully gapped d+id or nodal nematic ⇨ inconsistent
- L = 3 ⇨ Nodal f-wave ⇨ Consistent with lattice geometry

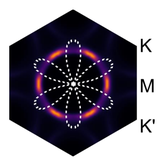




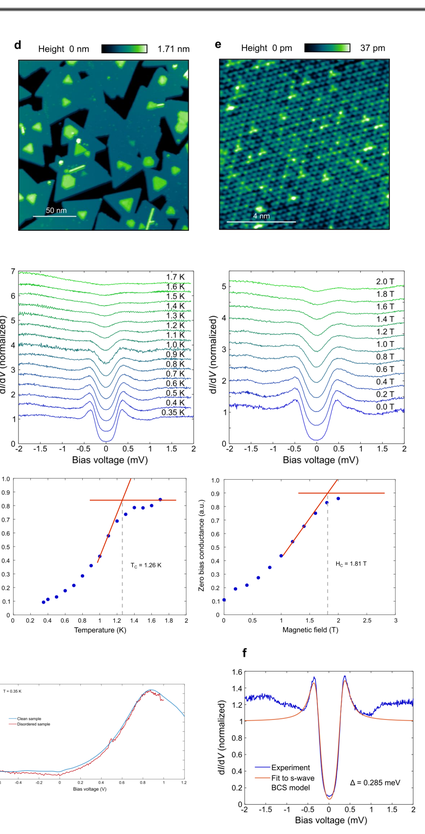
nodal f-wave model: $\rho(E) = \int_0^{2\pi} \left|\Re\left[\frac{E}{\sqrt{E^2-(\Delta\cos(\theta/3))^2}}\right]\right| d\theta$

$$\mathcal{H}^{f}_{SC} = \sum_{\mathbf{k}} \Delta^{\uparrow\uparrow}(\mathbf{k}) c^{\dagger}_{\mathbf{k},\uparrow} c^{\dagger}_{\mathbf{k},\downarrow} + \Delta^{\downarrow\downarrow}(\mathbf{k}) c^{\dagger}_{\mathbf{k},\downarrow} c^{\dagger}_{\mathbf{k},\uparrow} + \Delta^{\uparrow\downarrow}(\mathbf{k}) c^{\dagger}_{\mathbf{k},\uparrow} c^{\dagger}_{\mathbf{k},\uparrow} + \text{h.c.}$$

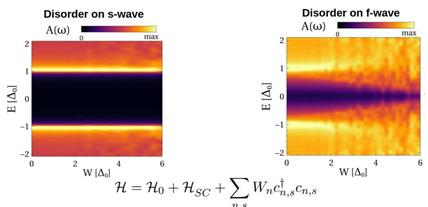
$\Delta^{\uparrow\downarrow}(\mathbf{k})$ nodal state is favoured



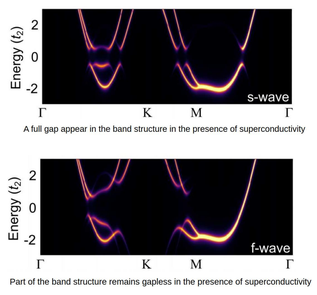
Observation of Disorder-induced emergence of s-wave gap



Suppression of nodal SC with disorder and emergence of s-wave gap



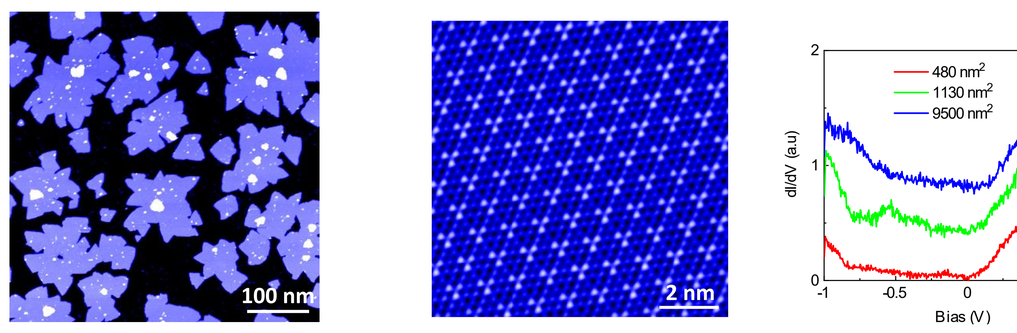
$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{SC} + \sum_{n,s} W_n c^{\dagger}_{n,s} c_{n,s}$$



A full gap appear in the band structure in the presence of superconductivity

Part of the band structure remains gapless in the presence of superconductivity

1H-$NbSe_2$/HOPG

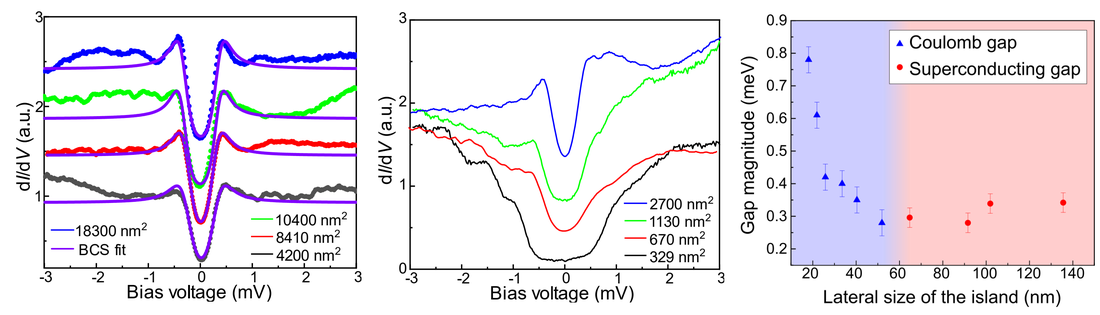


3x3 CDW

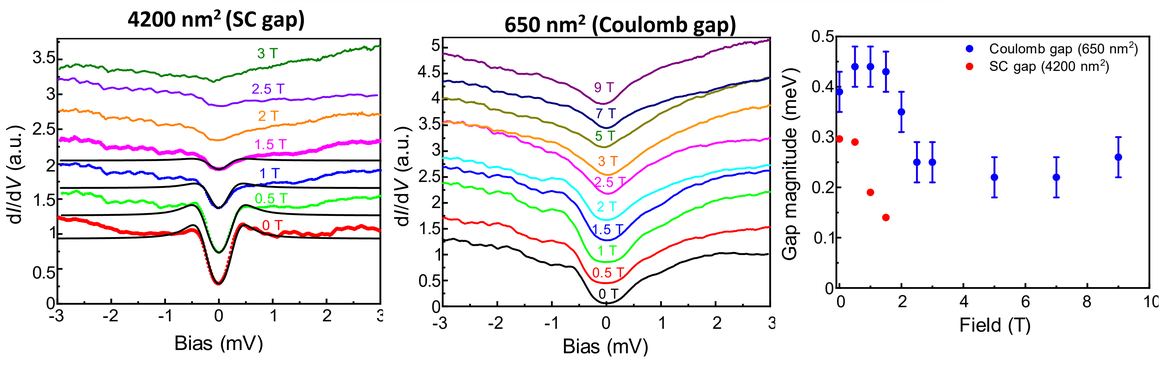
Nb d-band

- Lateral sizes: few tens of nm to several hundreds of nm
- Large variation in relative separations

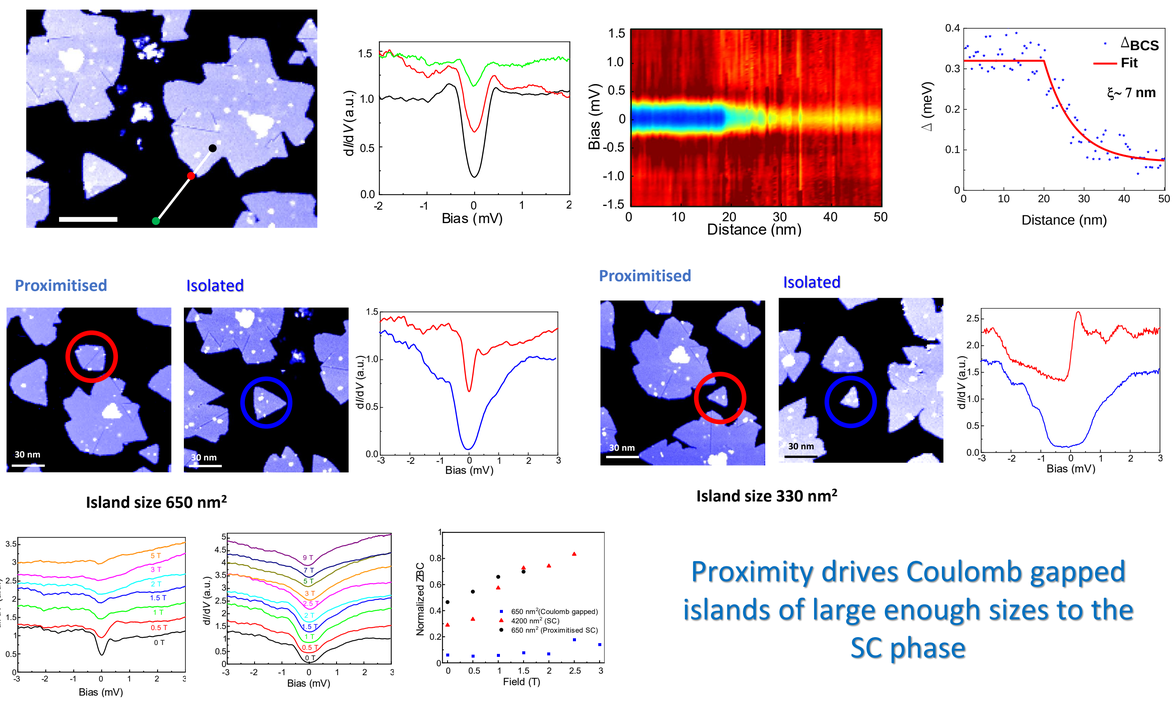
SC-Coulomb gap transition with size



Distinguishing SC and Coulomb gaps



Proximity induced transition

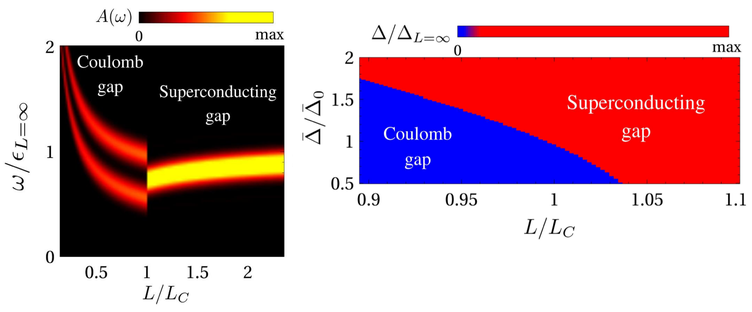


Proximity drives Coulomb gapped islands of large enough sizes to the SC phase

Summary and outlook

- 1H-$NbSe_2$ can be driven to a quantum phase transition from superconducting to a correlated regime. This transition occurs at a size (~60 nm) range several times larger than the coherence length of $NbSe_2$ (~7 nm). For correlated $NbSe_2$ samples close to the phase transition, superconducting proximity effect strongly impacts the ground state, pushing the system through the superconductor-correlated phase boundary. *Nano Lett.* 2022, 22, 5, 1845–1850
- 1H-TaS_2 shows nodal f-wave superconductivity with many body fluctuations and can be driven to a s-wave superconductivity with non-magnetic disorder. https://doi.org/10.48550/arXiv.2112.07316
- Our results suggests a role of electronic correlations for the emergence of both CDW and superconductivity besides the typical electron-phonon driven scenarios.
- These correlated states could be promoted in by gating, chemical doping or twist (Moire') engineering.

Theoretical Model



$$\mathcal{H} = \sum_i U \Psi^{\dagger}_{i,\uparrow} \Psi_{i,\uparrow} \Psi^{\dagger}_{i,\downarrow} \Psi_{i,\downarrow} - \sum_{i,j>i,s,s'} V \Psi^{\dagger}_{i,s} \Psi_{i,s} \Psi^{\dagger}_{j,s'} \Psi_{j,s'} + \mu \sum_{i,s} \Psi^{\dagger}_{i,s} \Psi_{i,s} + \bar{\Delta} \sum_i \Psi^{\dagger}_{i,\uparrow} \Psi^{\dagger}_{i,\downarrow} + H.C$$

$$U = U_0 + \frac{c_0}{L} \qquad A(\omega) = \sum_{i,s} \langle \Omega | \Psi_{i,s} \delta(\omega - H + E_0) \Psi^{\dagger}_{i,s} | \Omega \rangle$$

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