



# Doktorandský webinár 2021

ÚEF SAV

streda, 16. jún 2021

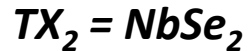
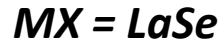


**Extreme charge transfer in the misfit layered  
compound  $(\text{LaSe})_{1.14}(\text{NbSe}_2)$**

**Ondrej Šofranko**

# Misfit materials

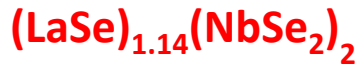
Naturally layered crystals  
Unit cell is stabilized by electron transport  
from MX part to TX<sub>2</sub>



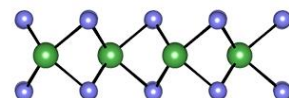
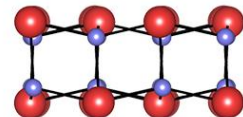
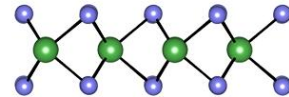
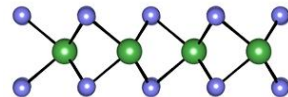
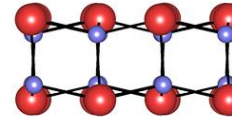
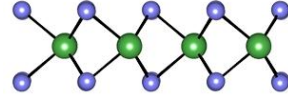
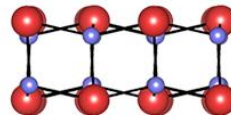
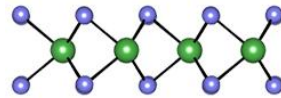
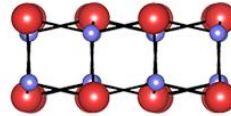
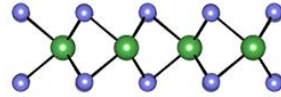
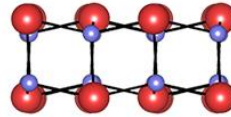
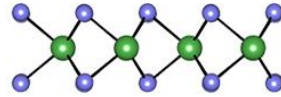
**Superconductors!**



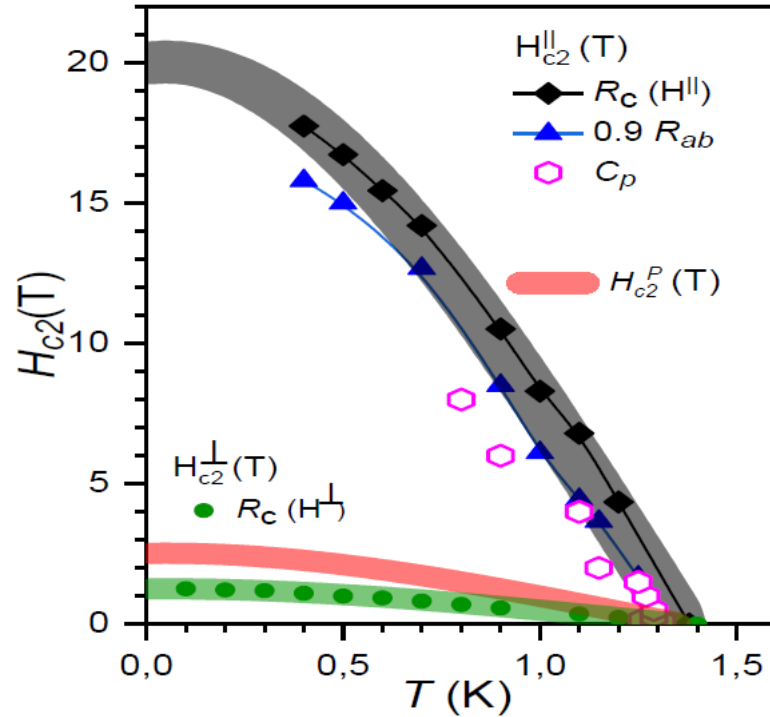
1Q1H;  $T_c \sim 1.2 K$



1Q2H;  $T_c \sim 5 K$



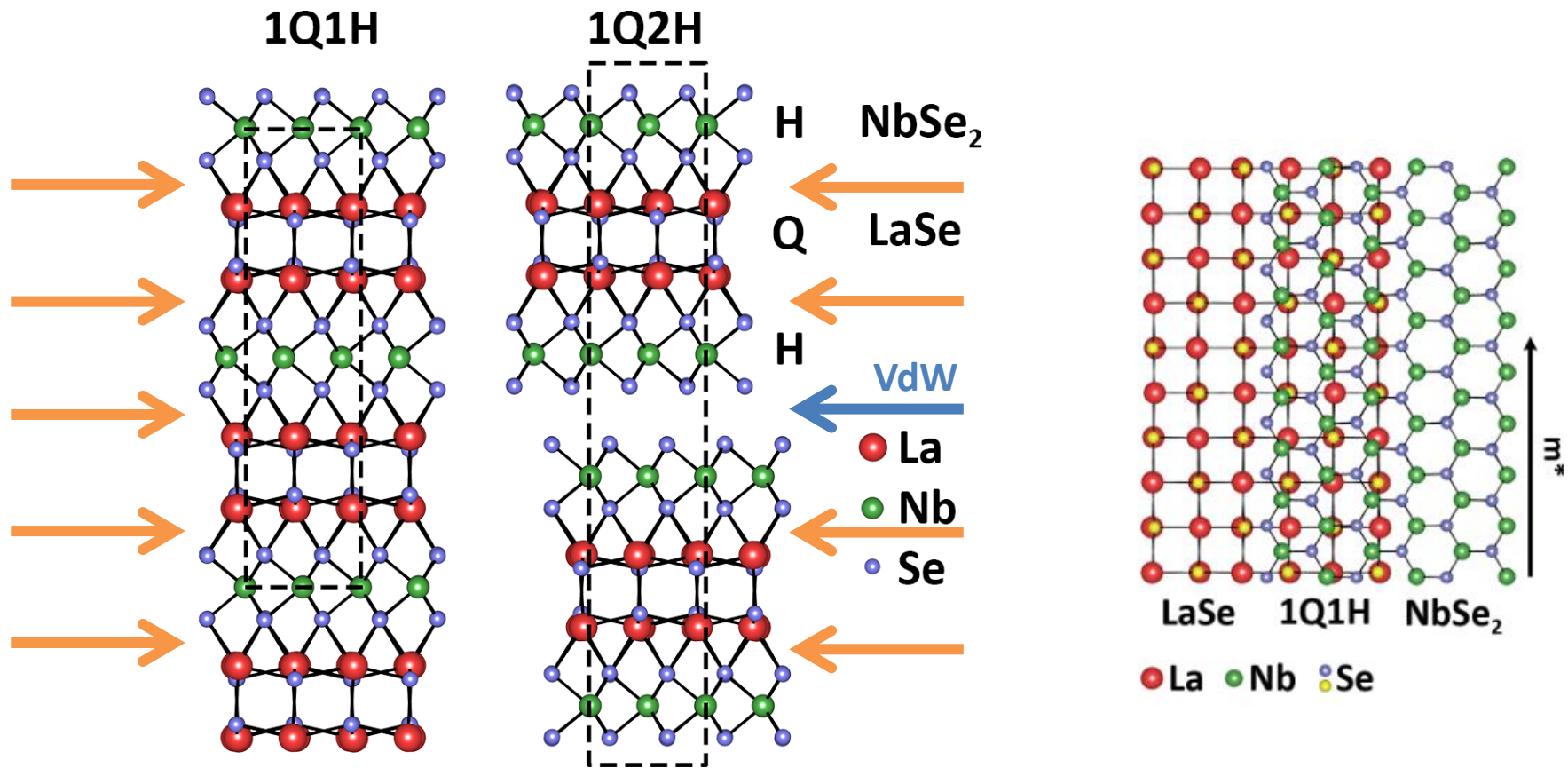
# Upper critical magnetic field



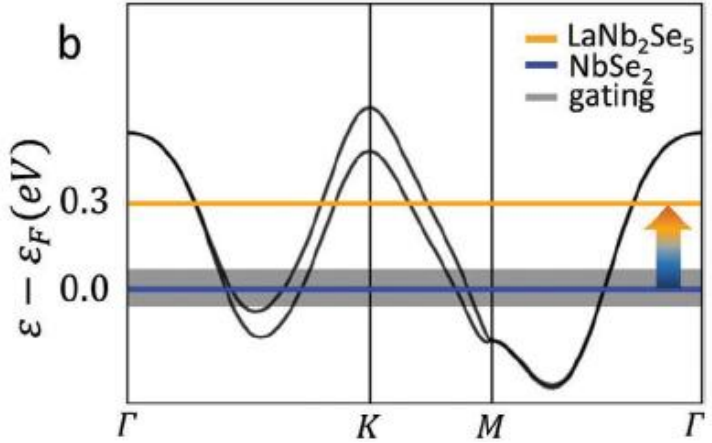
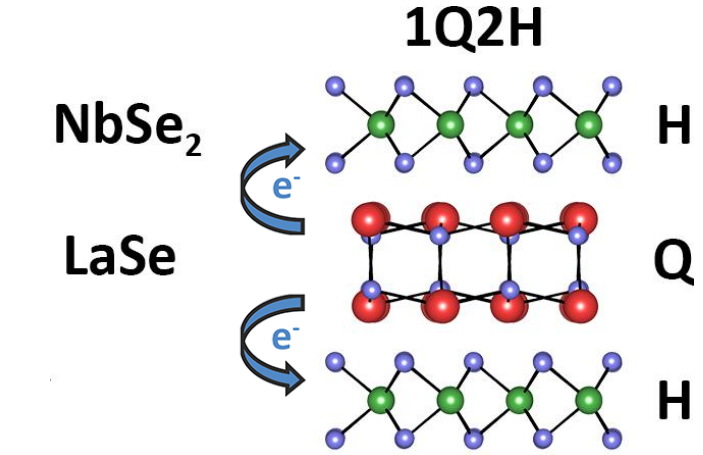
$$H_{c2//ab} = 10 \times H_p$$

$$H_{c2//ab} > 20 ? \times H_{c2//c}$$

Bulk superconductivity is confirmed by heat capacity measurements



Iono-covalent bonds



- Bulk VdW system consisting of weakly interacting 2D layers. These 2D layers are equivalent of extremely doped NbSe<sub>2</sub> monolayer.
- Such extreme doping is not achievable by other means (FET, K/Na deposition ... )
- Tunable by Pb → La substitution.
- ML NbSe<sub>2</sub> – is non-centrosymmetric system → electron spins are locked in out-of plane direction (Ising superconductivity) →  $H_{c2||ab} \gg H_p$

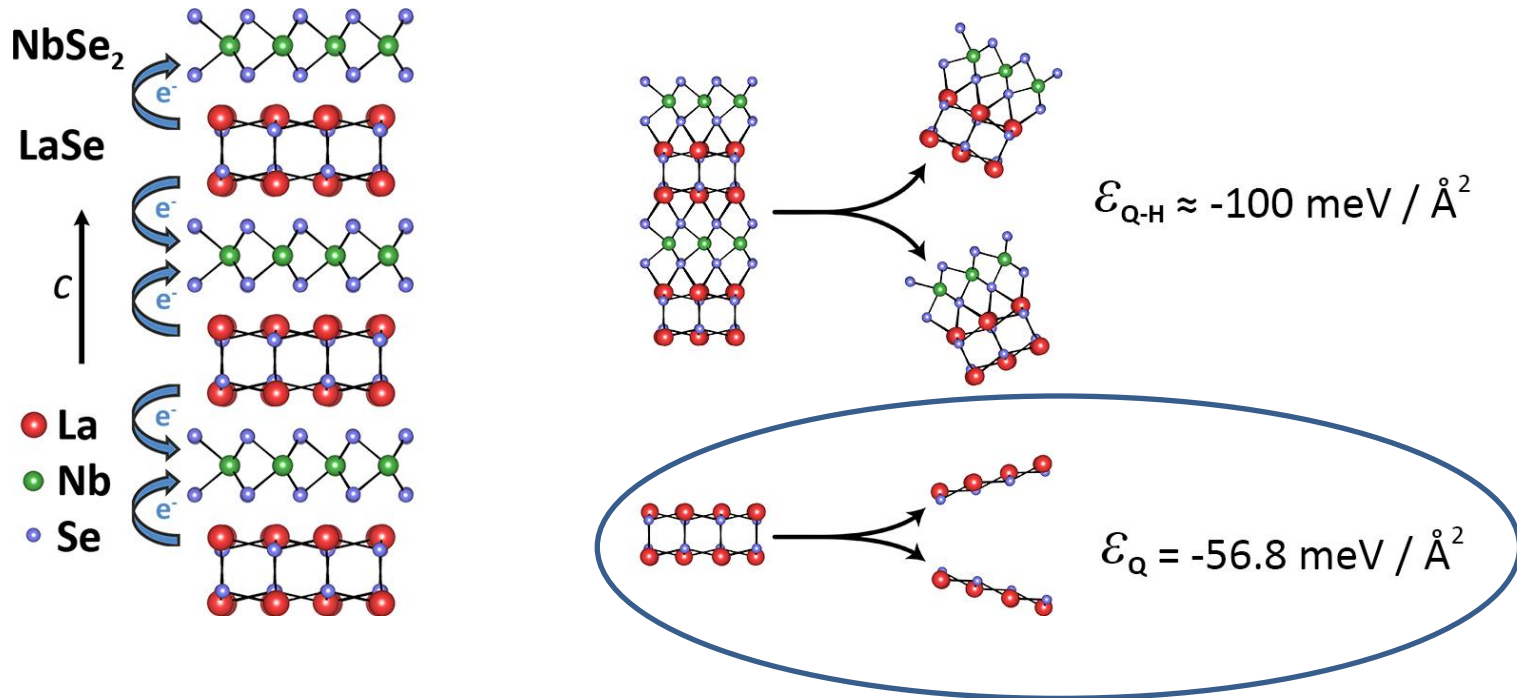
**ADVANCED FUNCTIONAL MATERIALS**

Full Paper | [Full Access](#)

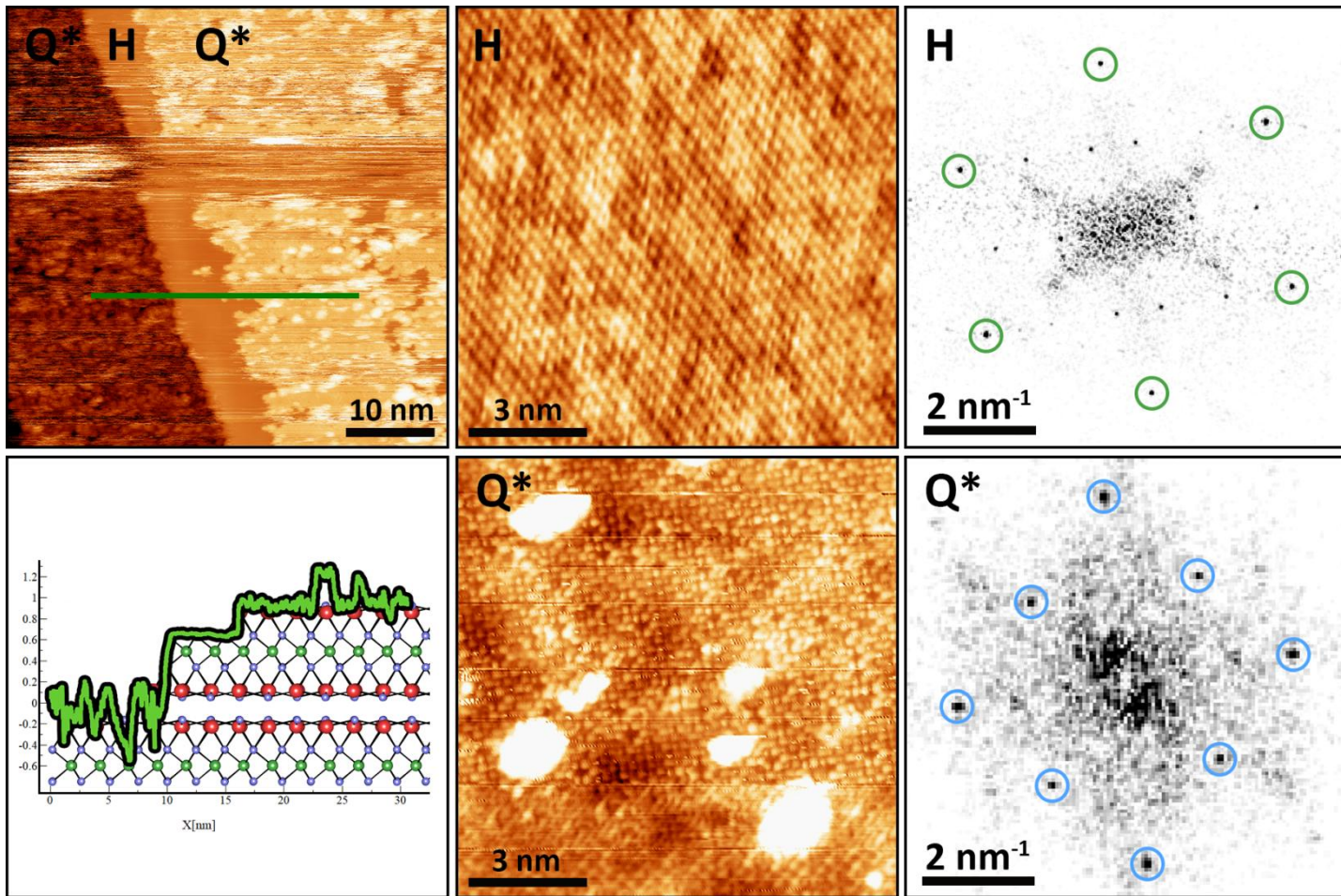
**Misfit Layer Compounds: A Platform for Heavily Doped 2D Transition Metal Dichalcogenides**

Raphaël T. Leriche, Alexandra Palacio-Morales, Marco Campetella, Cesare Tresca, Shunsuke Sasaki, Christophe Brun, François Debontridder, Pascal David, Imad Arfaoui, [Ondrej Šofranko](#), Tomas Samuely, Geoffroy Kremer, Claude Monney, Thomas Jaouen, Laurent Cario, Matteo Calandra, [Tristan Cren](#)  
 ... See fewer authors ^

## Structure and bonding 1Q1H



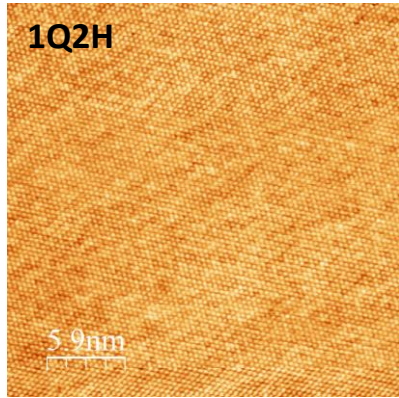
- Ionocovalent bonding (not vdW like 1Q2H)
- Breaking @Q into Q\*
- Q\* surface: unstable, ordered only at N2!



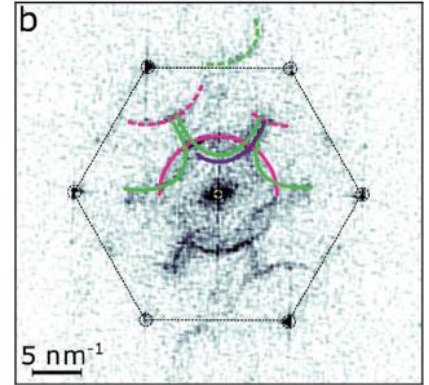
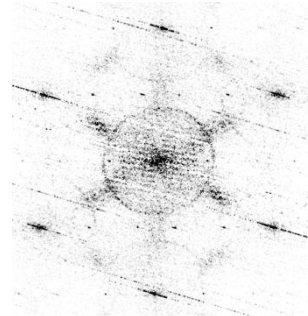
Fourier transform of atomically resolved surface is similar to diffraction methods (LEED)

# QuasiParticle Interference

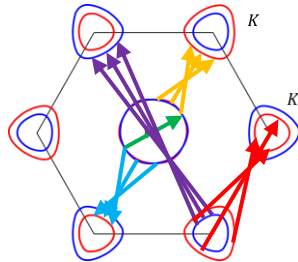
- Electrons can be described as Bloch wavefunctions + scattering  $\rightarrow$  interference  $\rightarrow$  standing wave pattern



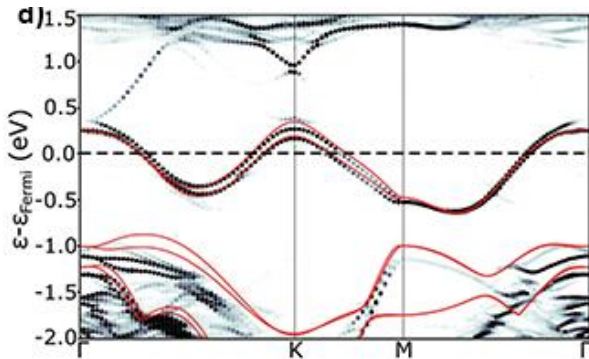
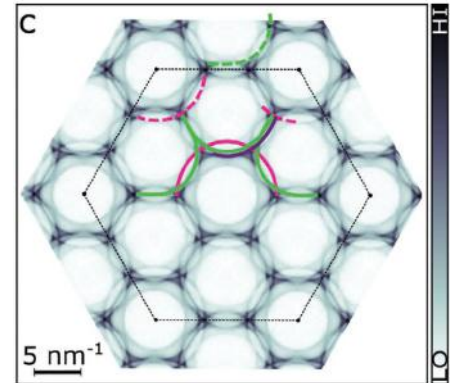
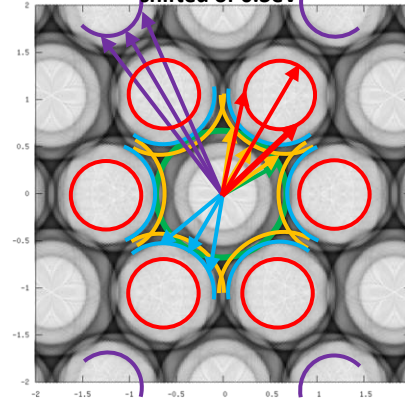
Fourier Transform



Fermi surface of monolayer NbSe<sub>2</sub> shifted of 0.3eV:



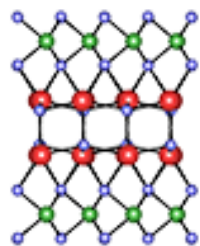
Joint-DOS of monolayer NbSe<sub>2</sub> shifted of 0.3eV



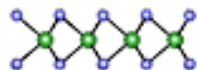


# H surface band structure – DFT & STS

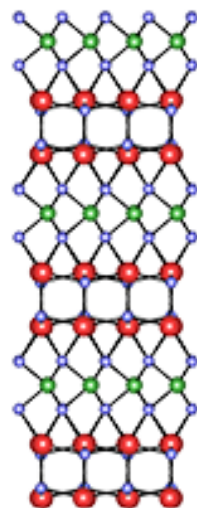
1Q2H



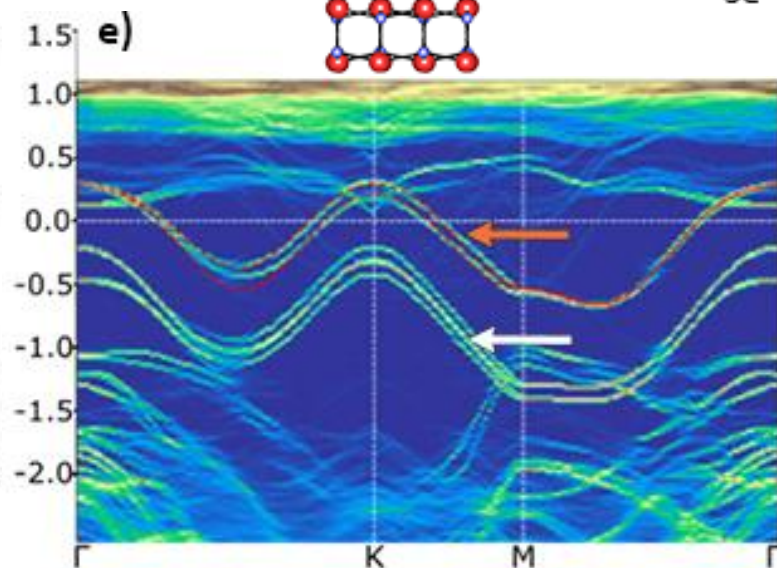
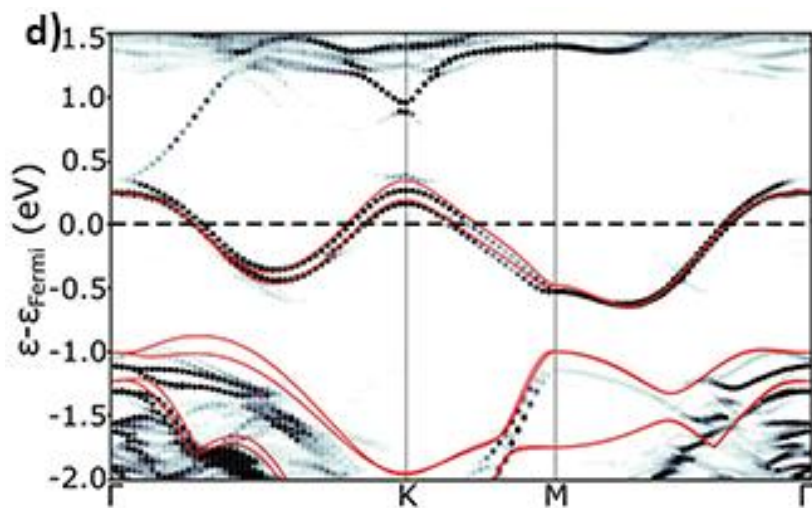
Monolayer NbSe<sub>2</sub>



1Q1H  
3 UC slab  
CC stacking

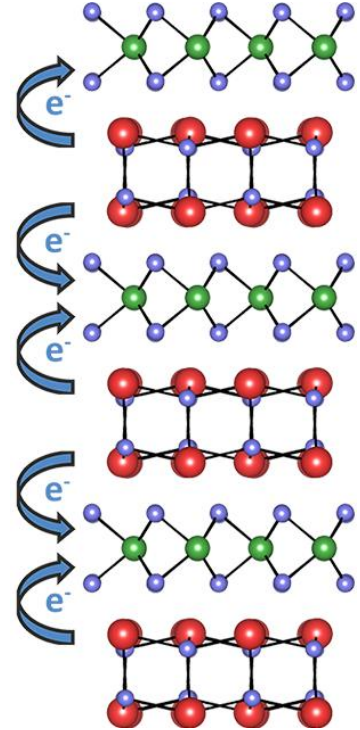
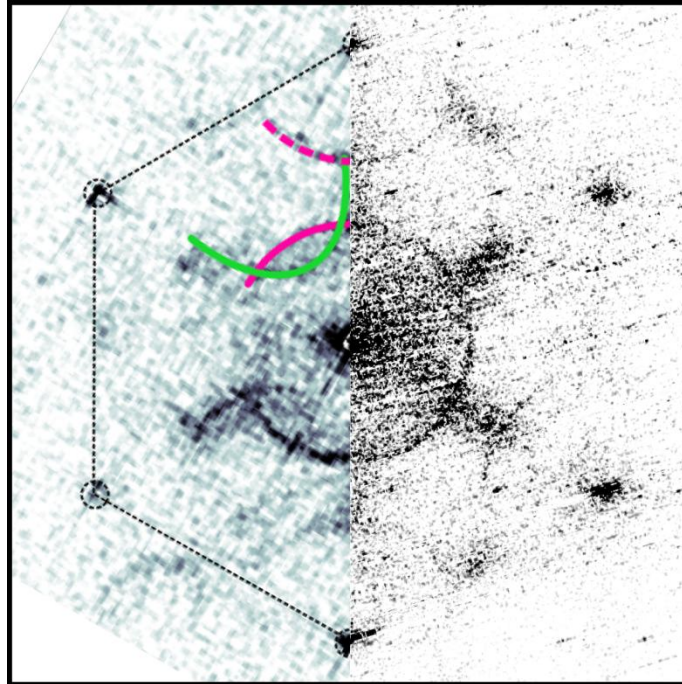
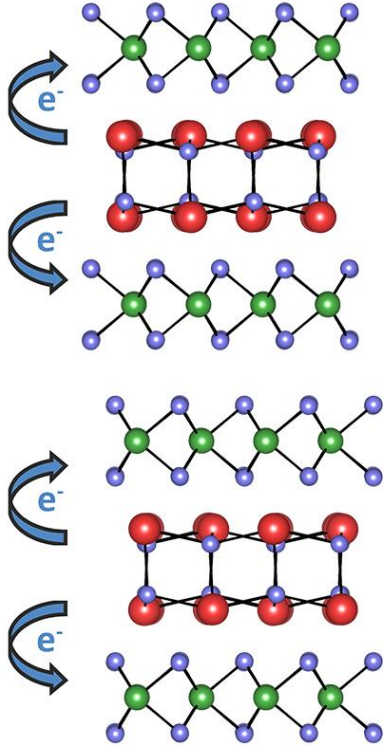


● La  
● Nb  
● Se



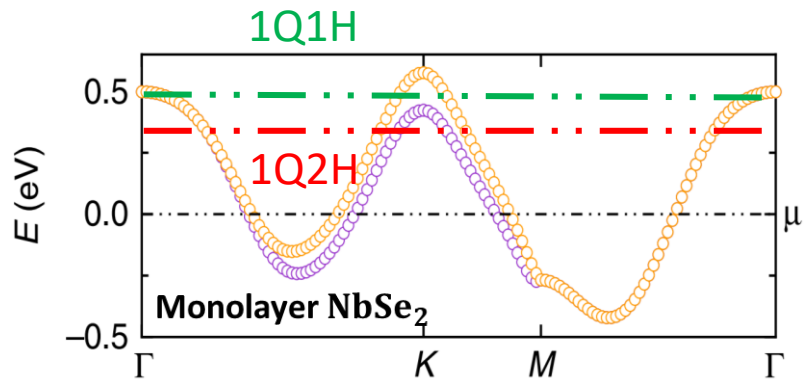
# Surface states, QPI

## 1Q2H – 1Q1H



## H + Q\* surface band structure ARPES

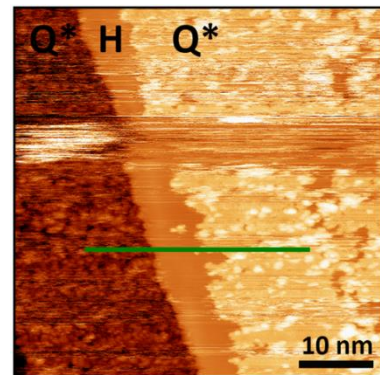
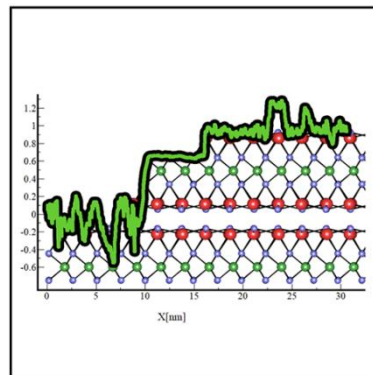
- Preliminary estimate: shift  $\sim 200\text{meV}$  compared to 1Q2H (H surface) due to Q\* “impurities” surface doping ???



Wen-Yu He, et al., *Communications Physics* 1, 40 (2018)

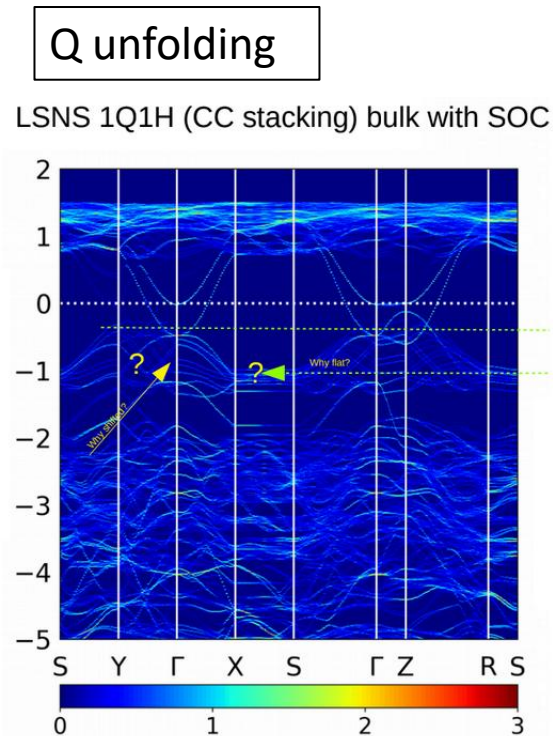
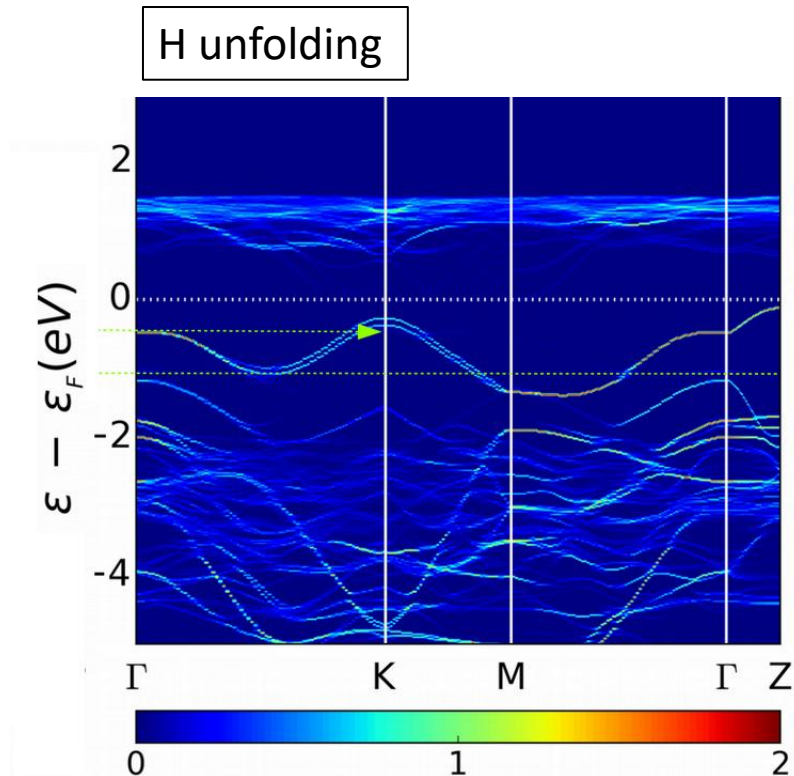
$$1Q2H = H$$

$$1Q1H = H + Q^*$$

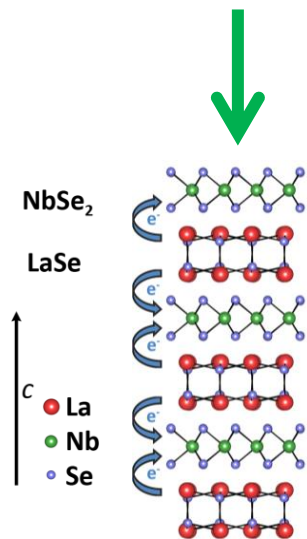


## DFT bulk 1Q1H

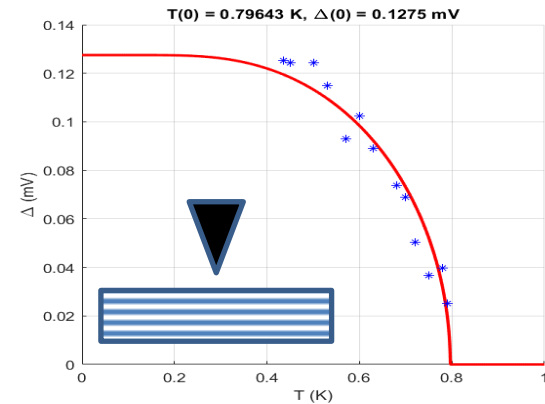
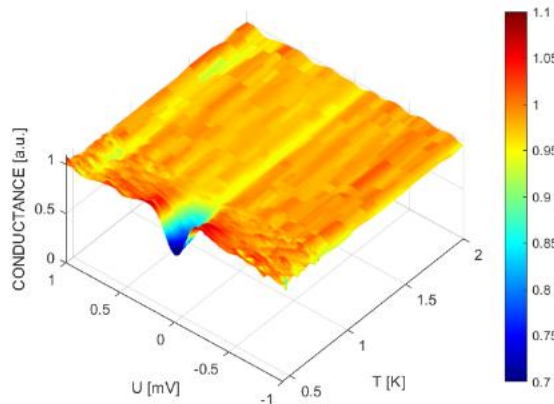
- 2x doping compared to 1Q2H
- NbSe<sub>2</sub> insulating
- LaSe conducting
- Bulk SC from **heat capacity**
- SC in LaSe



# Surface STM & STS



## Small surface superconducting gap



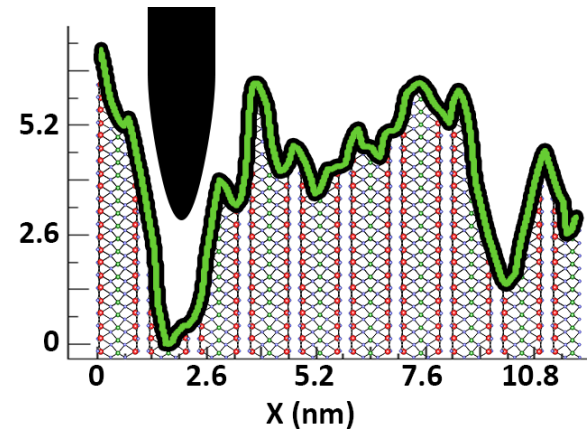
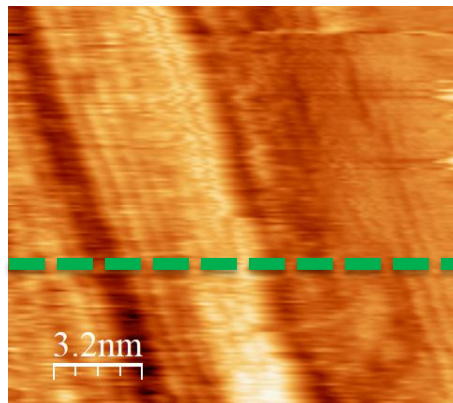
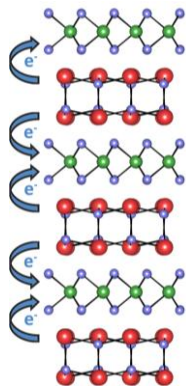
# Bulk STM & STS

NbSe<sub>2</sub>

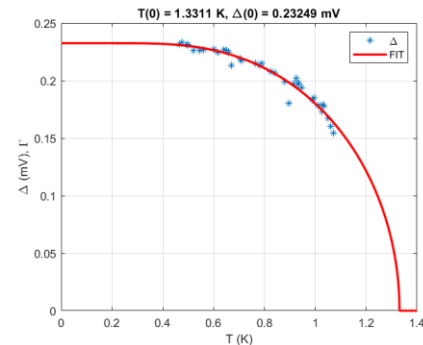
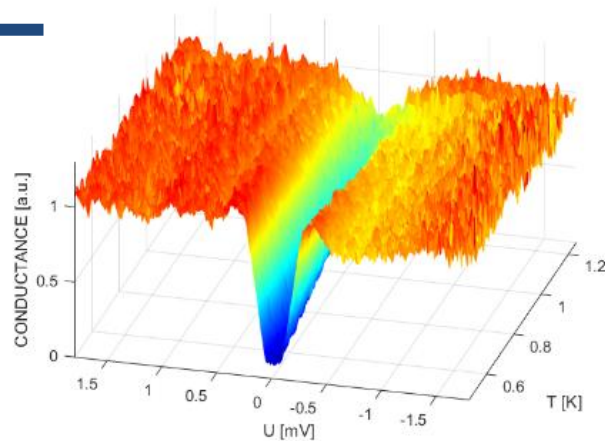
LaSe

c ↑

● La  
● Nb  
● Se



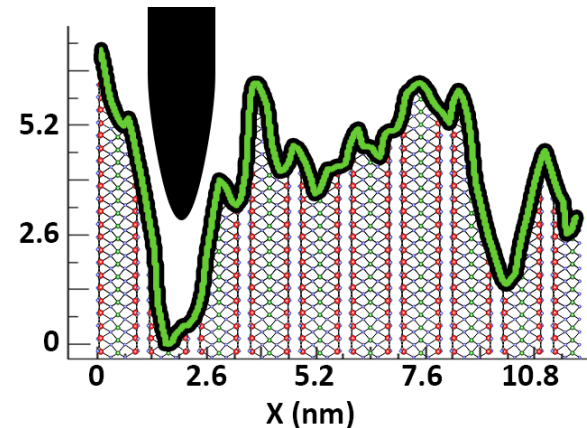
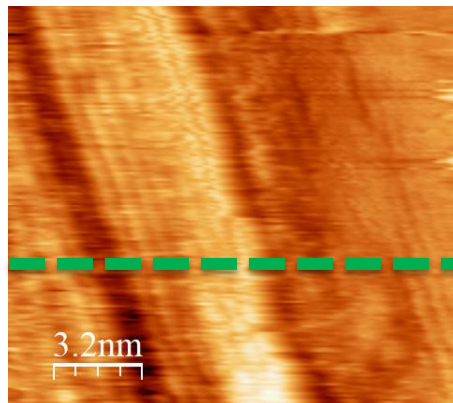
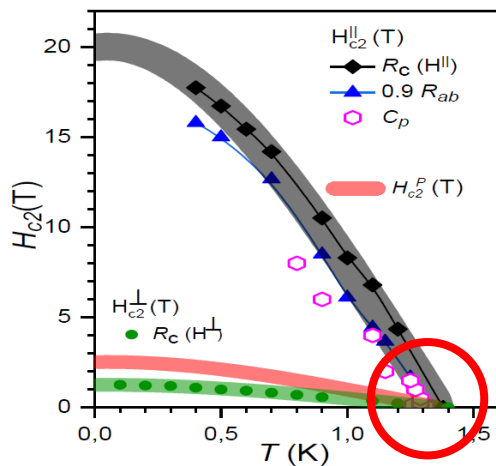
Large superconducting gap in the bulk



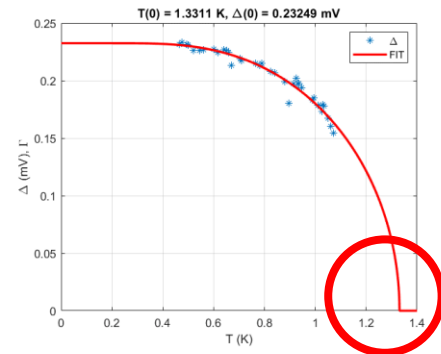
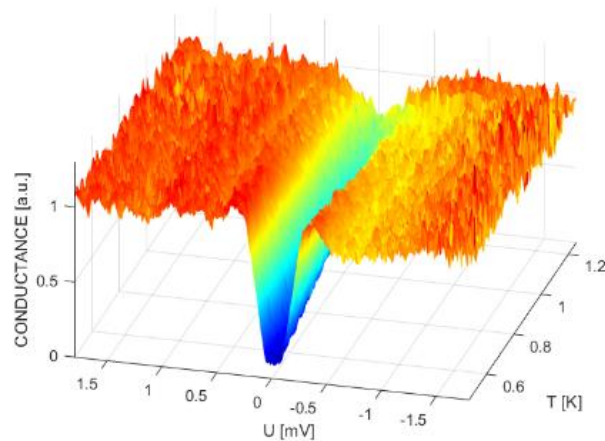
## Bulk STM & STS

- gap consistent with transport and **heat capacity**

Upper critical magnetic field

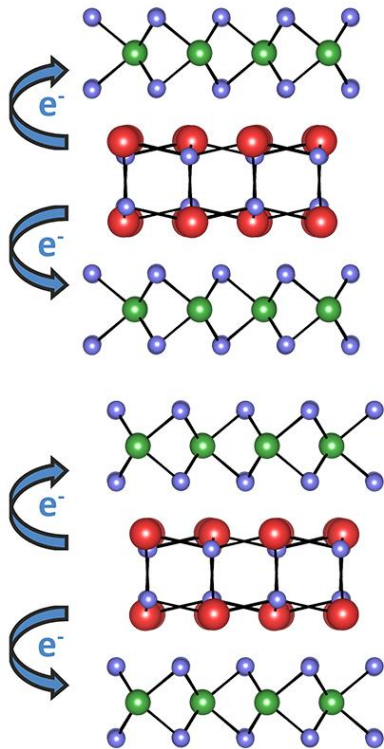


Large superconducting gap in the bulk



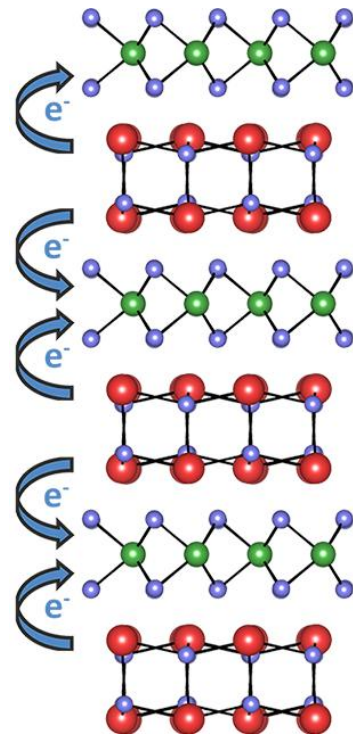
# Conclusions

## 1Q2H



- VdW crystal
- Decoupled doped NbSe<sub>2</sub> monolayers
- Bulk Ising SC from noncentrosymmetric NbSe<sub>2</sub> →  $H_{c2||ab} \gg H_p$

## 1Q1H



- Ionocovalent bonds between layers
- Even higher doping → superconducting LaSe is decoupled by insulating NbSe<sub>2</sub> monolayers
- LaSe is centrosymmetric → why is  $H_{c2||ab} \gg H_p$  ?



# Acknowledgments

Theoretical support



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M. Gmitra



## Collaborators

T. Cren



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M. Calandra



M. Campetella



C. Tresca



F. Debontridder



P. David



I. Arfaoui



## Sample preparation



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S. Sasaki

## ARPES



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C. Monney

T. Jaouen

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Thank you for your attention!