Ab initio study of the Van der Waals Superconductor $NbSe_2$

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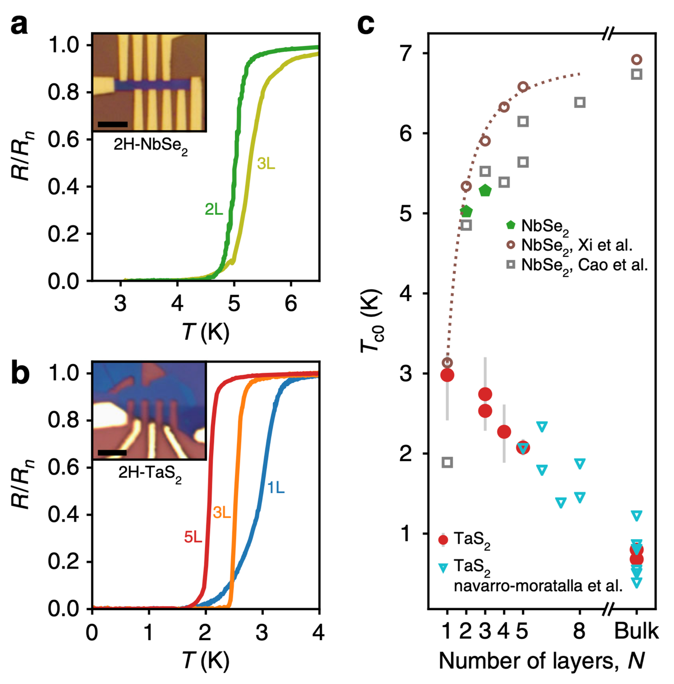
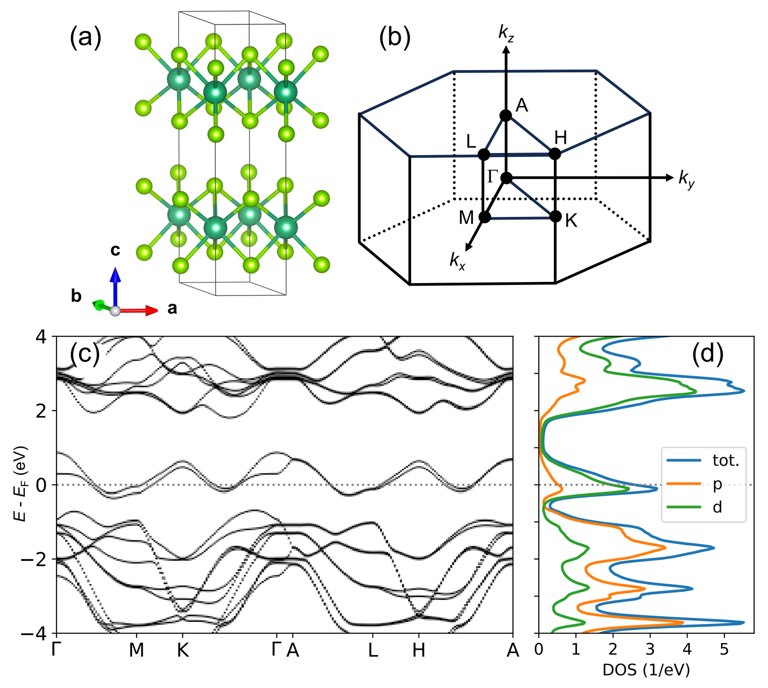
Introduction

Transition metal dichalcogenides (TMDCs) are a very versatile material class in which many physical phenomena can be found [1]. These phenomena range from a topological electronic structure in Weyl and Dirac semimetals to magnetic and even superconducting systems and charge-density waves (CDWs). Different van der Waals (vdW) materials can also be combined easily due to the intrinsic vdW stacking. The TMDC $NbSe_2$ is an example of a superconducting TMDC which shows the unconventional Ising superconductivity up to T_C=7K that is particularly robust against magnetic fields in certain directions [1, 2].

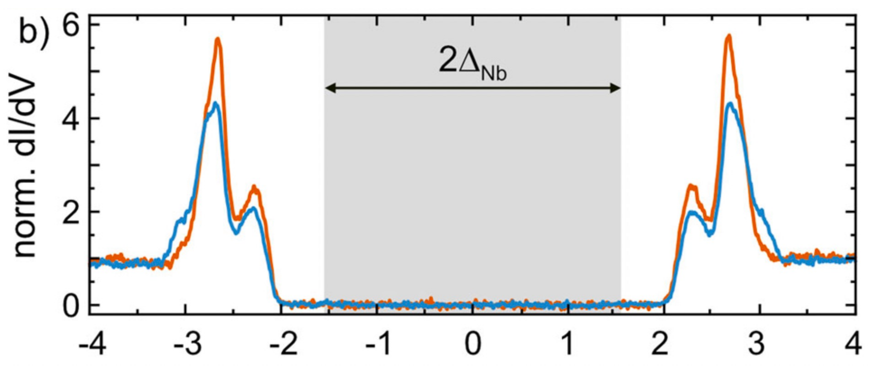
Superconducting Temperature of different thickness of **$NbSe_2$** [3]



Materials Data on **$NbSe_2$** by Materials Project [5]



Superconductivity Gap size detected by Scanning Tunneling Microscopy of NbSe2 [2].



Method

Using the recent Bogoliubov-de Gennes extension to the Korringa-Kohn-Rostoker Green's function method in JuKKR code[4], we investigate the electronic structure of superconducting NbSe2 [5].

$$H_{\text{BdG}}(\boldsymbol{x}) = \begin{pmatrix} -\nabla^2 - E_F + V_{\text{eff}}(\boldsymbol{x}) & 0 \\ 0 & \nabla^2 + E_F - V^*_{\text{eff}}(\boldsymbol{x}) \end{pmatrix} + \begin{pmatrix} 0 & \mathcal{D}_{\text{eff}}(\boldsymbol{x}) \\ \mathcal{D}^*_{\text{eff}}(\boldsymbol{x}) & 0 \end{pmatrix},$$

$$\mathcal{D}_{\text{eff}}(x) = \lambda\chi(x).$$

semiphenomenological coupling constant (electron-phonon coupling constant)

The Coherent Potential Approximation is employed to treat the effects of disorder on the electronic structure. It extends the KKR formalism to include disordered systems assuming an effective medium.

Introducing the effective medium t_i, here τ_{ii} is the effective medium scattering path operator and Δ_{ii} the hybridization function.

$$\tau_{ii} = [(t_i)^{-1} - \Delta_{ii}]^{-1},$$

place real impurity scatterer in the effective medium:

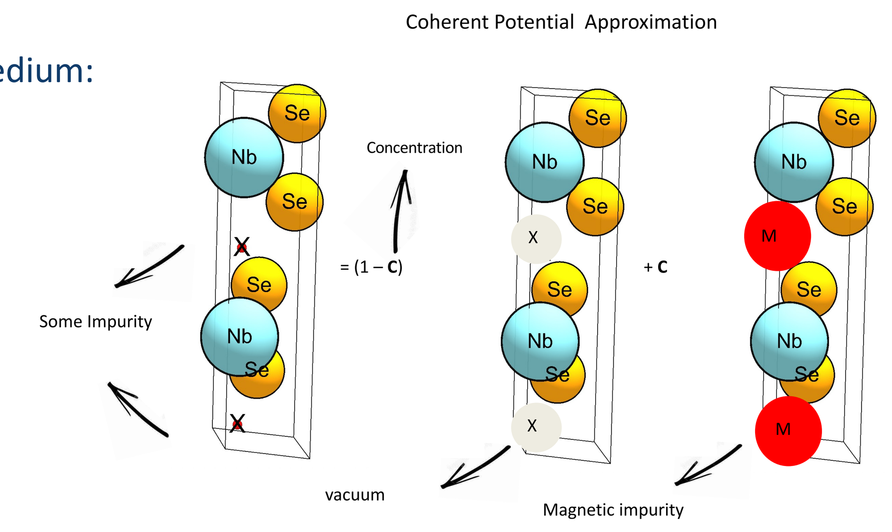
$$\tau^{\alpha} = [(t^{\alpha})^{-1} - \Delta]^{-1},$$

with:

$$\tau = \frac{1}{\Omega_{BZ}} \int dk [(\bar{t})^{-1} - G^0(k)]^{-1},$$

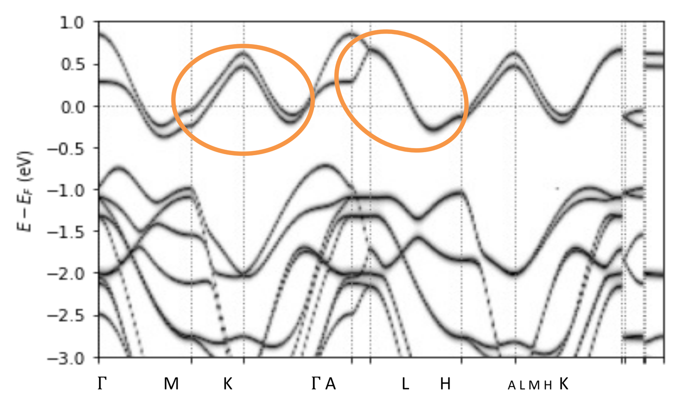
Then solve it self-consistently:

$$\langle \tau^{\alpha} \rangle = \tau.$$

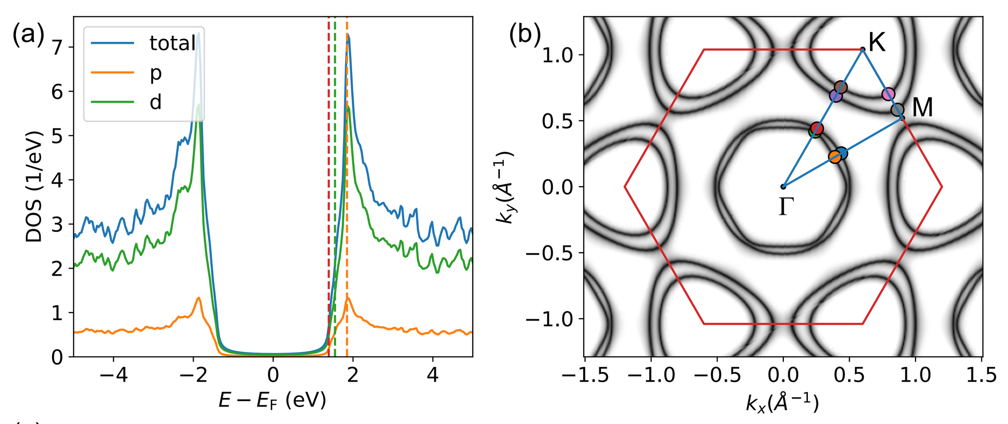


Superconducting Band Structure

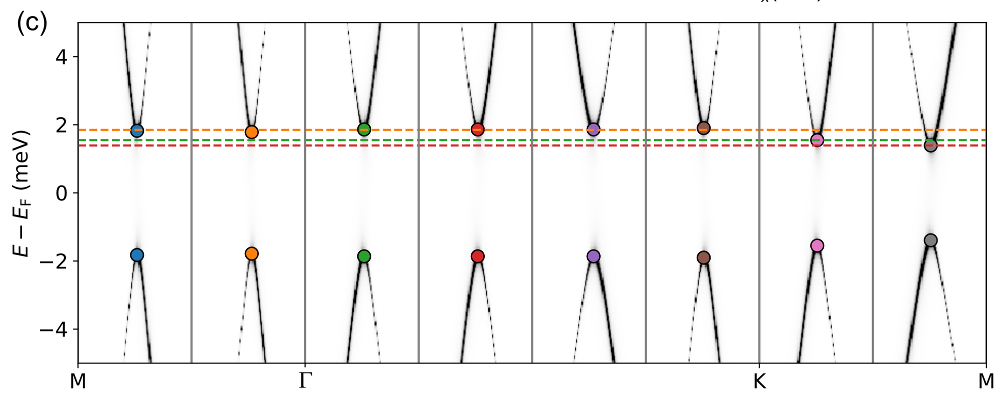
Band Structure and Density of normal states of $NbSe_2$
Strong Spin-Orbit Coupling can cause degenerecies



a) Superconducting density of states
b) Fermi surface [6]



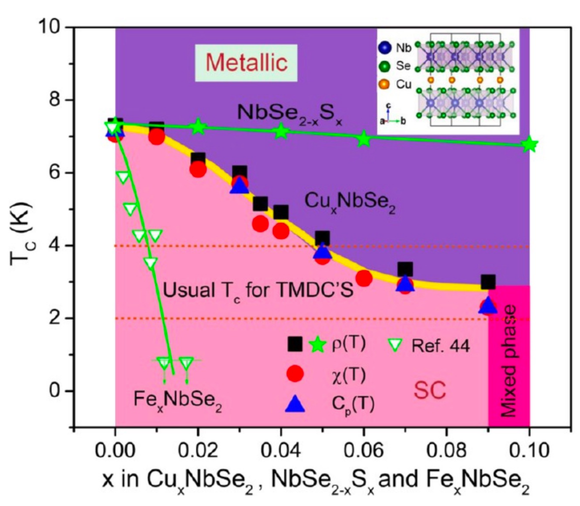
c) Superconducting electronic Gap for the points marked in b [6]



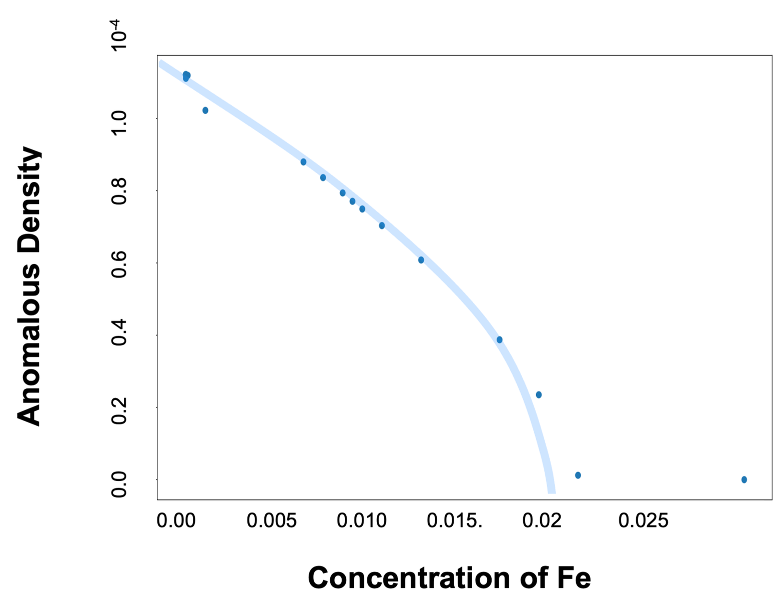
Magnetic Impurity

AiiDA JuKKR *Ab initio* calculations (AiiDA-KKR) Quantum mechanical model

The change of Anomalous Density with changing the impurity concentration looks Similar to the Superconducting Temperature behaviour when impurity concentration changes.



Experimental Results of Magnetic doping in **$NbSe_2$** [7]



Planned Work

- Study other defects, Majorana chains, and magnetic chains
- Exploring (if any) the topological properties
- Creating hetrostructures using vdW stacking
- We hope this study may shine some light on realization of Majorana zero modes

References

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[5] P. Rüßmann and S. Blügel, PRB 105, 125143 (2022)
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[7] Huixia Luo, *et al., Chem. of Materials 29* (8) (2017)