Coulomb Interaction in Transition Metal Dichalcogenides

Effects on Many-Body Instabilities

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3: Department of Physics and Astronomy, University of Southern California

What about U?, ICTP, October 17, 2016

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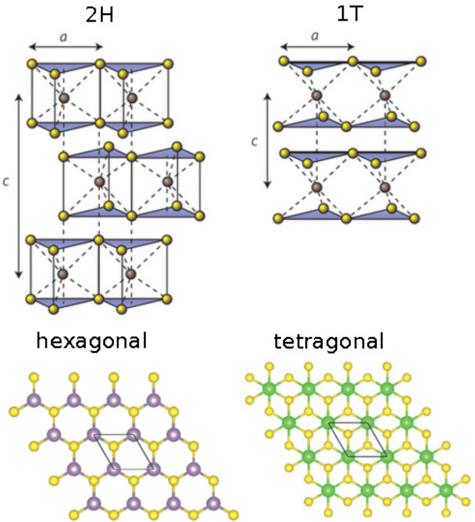
Outline

- Transition Metal Dichalcogenides
  - Many-Body Effects
  - Theoretical Description
- Interplay of Screening and Superconductivity
  - Conventional and Unconventional Superconductivity
- Conclusions

Transition Metal Dichalcogenides

- TX_2
  - T: Mo, W, Nb, ...
  - X: S, Se, Te
- structure: 2H, 1T
- semiconducting or metallic



- sensitive to the environment
- no environmental screening

$\Rightarrow$ enhanced Coulomb interaction

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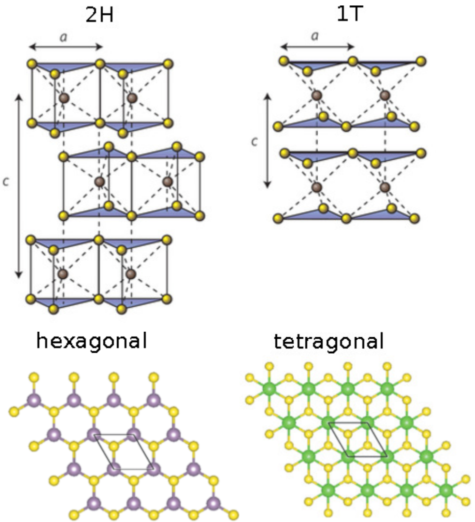

[right] Wang et al., Nat. Nano, 7 (11), 699

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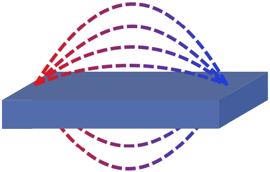

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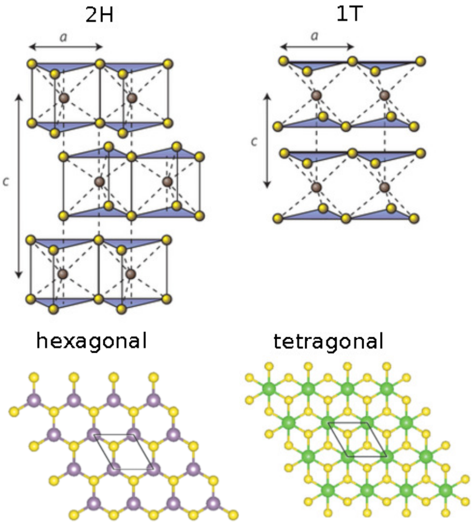

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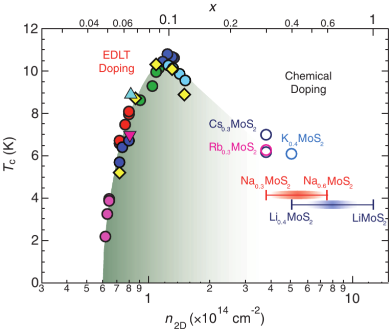
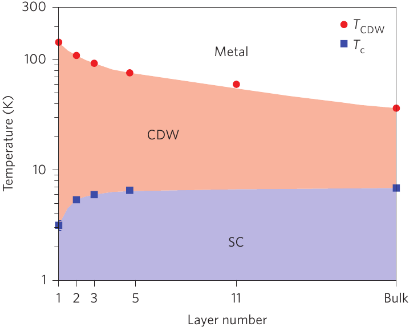
Many-Body Instabilities in TMDCs

Superconductivity in doped MoS_2

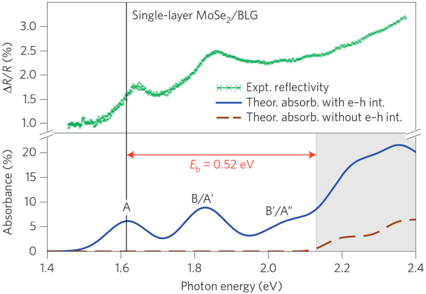


Charge Density Waves in (metallic) $NbSe_2$

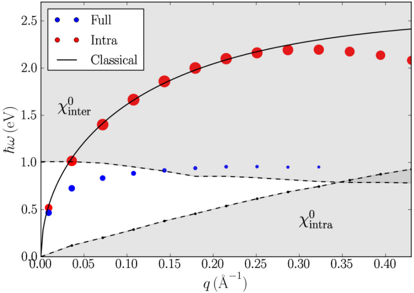


Many-Body Excitations in TMDCs

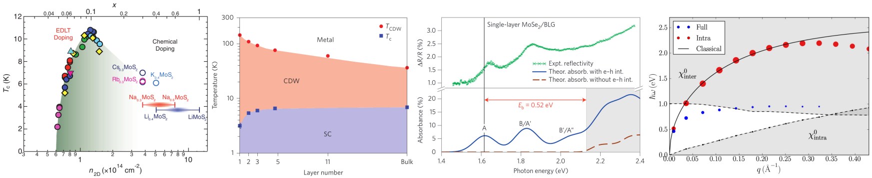
Excitons in semiconducting $MoSe_2$



Plasmons in metallic TX_2



Many-Body Effects in TDMCs



⇒ instabilities and excitations strongly depend on doping levels, thicknesses, and environments

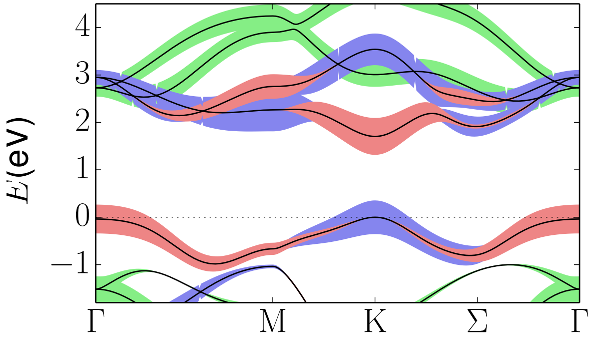
⇒ adequate descriptions need

- precise electronic dispersions
- accurate Coulomb interactions

involving doping and environmental screening effects

TMDC Model: MoS_2

$$H = \sum_{\langle ij \rangle,\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow} + \sum_{i \neq j \sigma \sigma'} V_{ij} c^\dagger_{i\sigma} c_{i\sigma} c^\dagger_{j\sigma'} c_{j\sigma'}$$



red: Mo d_{z^2}
blue: Mo $d_{xy} + d_{x^2-y^2}$
green: Mo $d_{xz} + d_{yz}$

$\Rightarrow$ use Mo d_{z^2}, d_{xy}, and $d_{x^2-y^2}$ orbitals to evaluate $t_{\alpha\beta}$ and $U_{\alpha\beta\gamma\delta}$

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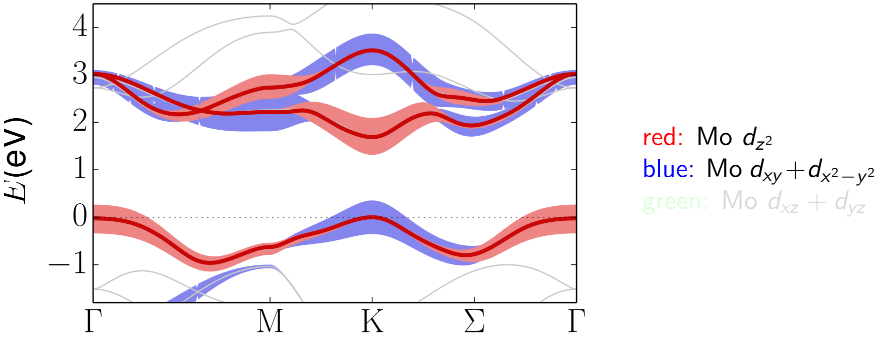

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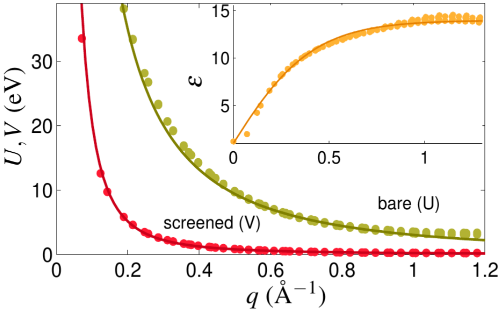
TMDC Model: MoS_2 - Coulomb Interactions

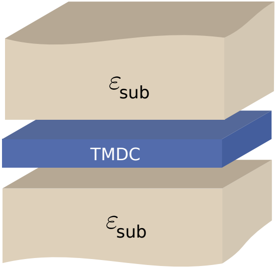


- extract $U(q)$, $V(q)$ and $\varepsilon(q)$ from GW calculations
- in Mo d_{z^2}, d_{xy}, $d_{x^2-y^2}$ basis
- $\varepsilon(q \to 0) \to 1$: typical 2D screening in semiconductors

$\Rightarrow$ interband screening

[right] Steinhoff, MR et al., Nano Lett. 14, 3743 (2014)

TMDC Model: MoS_2 - Coulomb Interactions

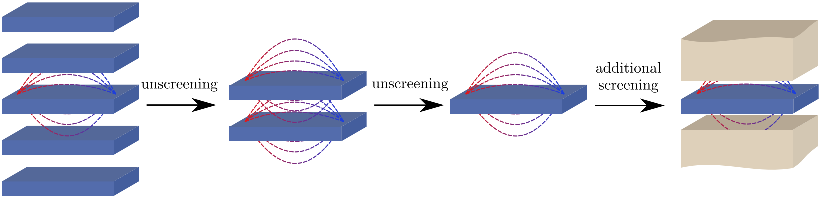


- dielectric environment yields additional screening channels
- reduces "internal" Coulomb interaction

either: redo ab initio calculations including surrounding material

or: use Wannier Function Continuum Electrostatics!

Wannier Function Continuum Electrostatics



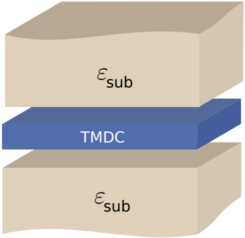
MR et al., PRB 92, 085102 (2015)

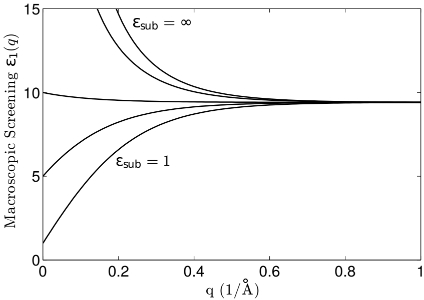
- changing the dielectric environment is a macroscopic electrodynamic problem
- normally hard to combine with atomistic quantum mechanical description

$\Rightarrow$ utilize Wannier basis $\{\tilde{\alpha}, \tilde{\beta}\}$

- macroscopic screening is controlled by a single element of the dielectric matrix $\varepsilon_{\tilde{\alpha},\tilde{\beta}}(q)$
- changing this element changes the environmental screening

TMDC Model: MoS_2 - Coulomb Interactions





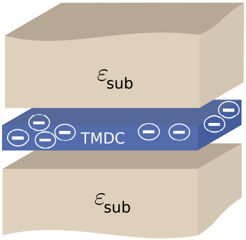
- use Wannier Function Continuum Electrostatics (WFCE) to include environmental screening

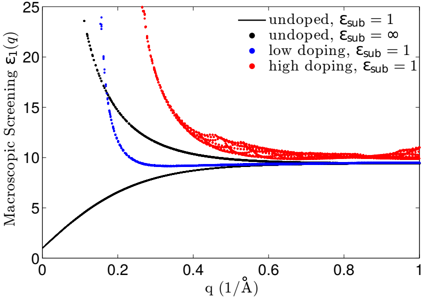
$$\varepsilon_{\text{inter}}^{\text{env}}(q) = \varepsilon_\infty \frac{1 - \beta_1 \beta_2 e^{-2\,q\,d}}{1 + (\beta_1 + \beta_2) e^{-q\,d} + \beta_1 \beta_2 e^{-2\,q\,d}} \qquad \beta_i = \frac{\varepsilon_\infty - \varepsilon_{\text{sub,i}}}{\varepsilon_\infty + \varepsilon_{\text{sub,i}}}$$

$\Rightarrow$ interband and environmental screening

[right] Schönhoff, MR et al., PRB 94, 134504 (2016)

TMDC Model: MoS_2 - Coulomb Interactions





- evaluate RPA bubble to add doping-induced intra-band screening

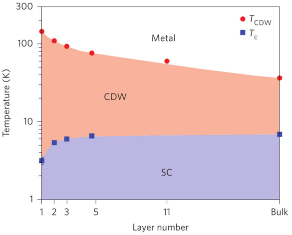
$$\varepsilon_{\mathrm{full}}(\mathbf{q},\omega) = 1 - V^{\mathrm{env}}_{\mathrm{inter}}(q)\Pi(\mathbf{q},\omega) \qquad V^{\mathrm{env}}_{\mathrm{inter}}(q) = \left[\varepsilon^{\mathrm{env}}_{\mathrm{inter}}(q)\right]^{-1} U(q)$$

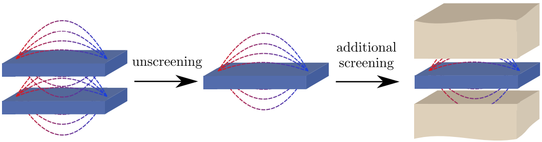
$\Rightarrow$ interband, intraband, and environmental screening

$$W(\mathbf{q},\omega) = \left[\varepsilon_{\mathrm{full}}(\mathbf{q},\omega)\right]^{-1} V^{\mathrm{env}}_{\mathrm{inter}}(q)$$

[right] Schönhoff, MR et al., PRB 94, 134504 (2016)

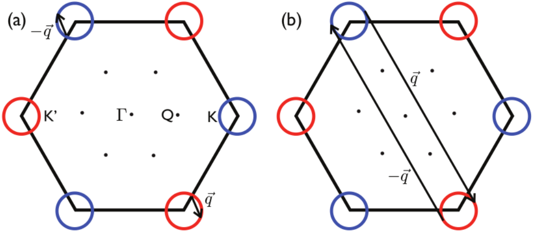
Interplay of Screening and Superconductivity





[left] Xi et al., Nat. Nano. 10, 765 (2015)

Unconventional Superconductivity in Doped MoS_2



$\Rightarrow$ no phononic glue needed for

$\mu_{\text{inter}} > \mu_{\text{intra}}$

[1] Roldan et al., PRB 88, 054515 (2013)

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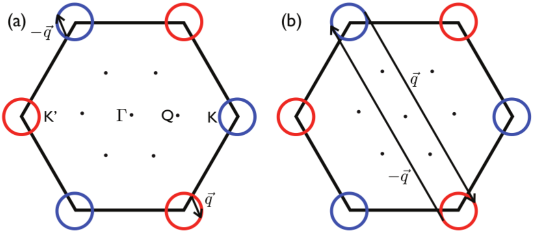

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$\Uparrow$

averaged Coulomb interaction

$$\mu = \frac{1}{N(E_F)} \sum_{\mathbf{kk}'} W(\mathbf{k}-\mathbf{k}', \omega = 0)\delta(\epsilon_{\mathbf{k}} - E_F)\delta(\epsilon_{\mathbf{k}'} - E_F)$$

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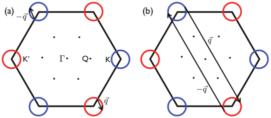

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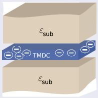

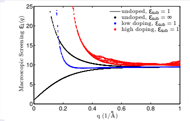

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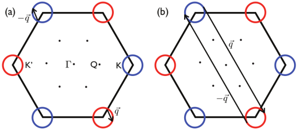

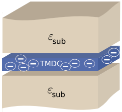

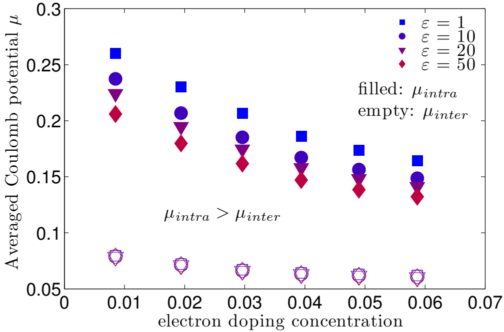

- ε_{sub} influence to ...
  - μ_{intra} strong
  - μ_{inter} negligible
- $\mu_{intra} > \mu_{inter}$

$\Rightarrow$ no Coulomb-driven unconventional superconductivity

$\Rightarrow$ additional renormalizations or spin fluctuations needed

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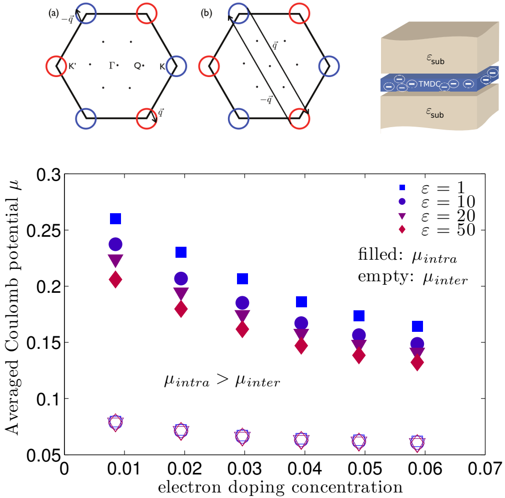

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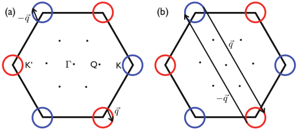

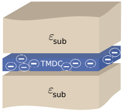

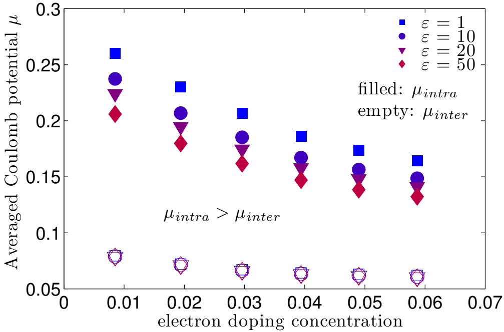

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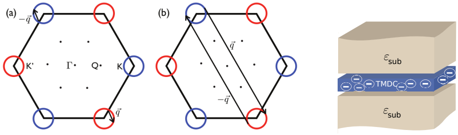

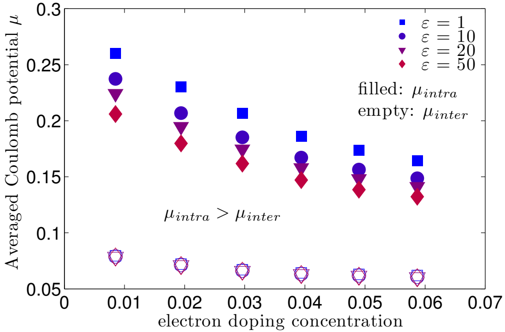

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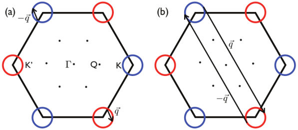

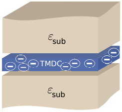

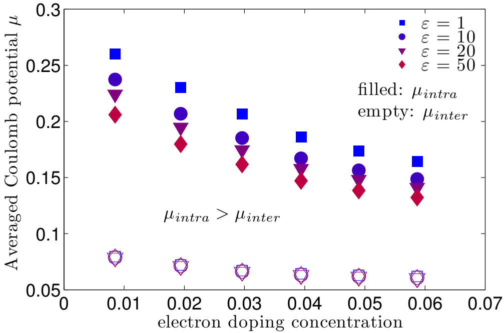

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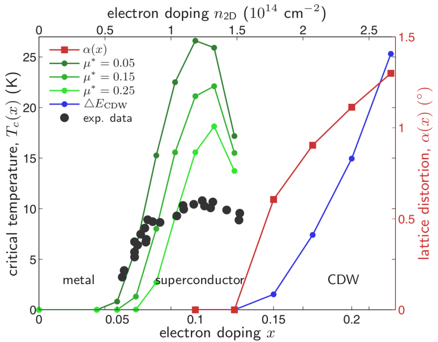

- Eliashberg / Allen-Dynes theory

$$T_c = \frac{\hbar\omega_{\log}}{1.2k_B} \exp\left[\frac{-1.04(1+\lambda)}{\lambda(1-0.62\mu^*)-\mu^*}\right]$$

$\omega_{\log}$: typical ph. frequency
λ : el.-ph. coupling
μ^* : Coulomb pseudo potential

- significant T_c for $\lambda/3 > \mu^*$
- fits reasonable well
- ... but: What about μ^*?

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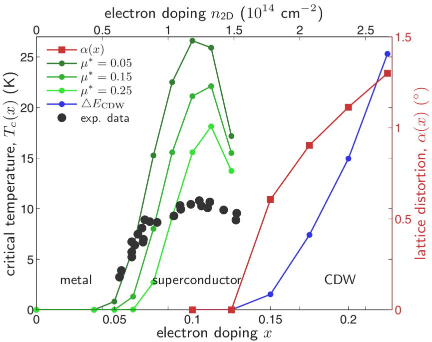

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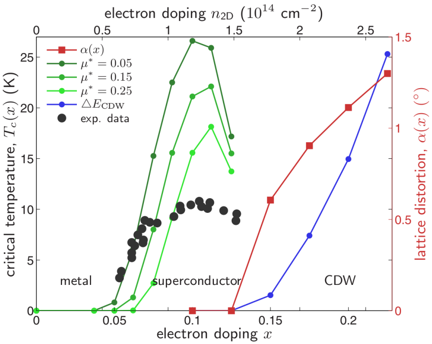

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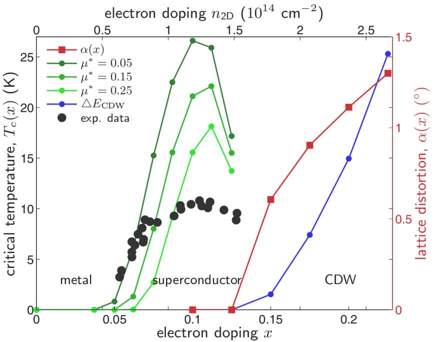

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Coulomb pseudo potential

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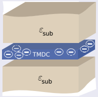

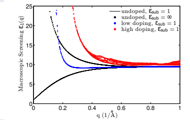

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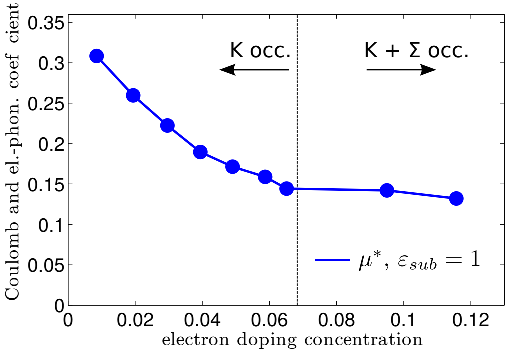

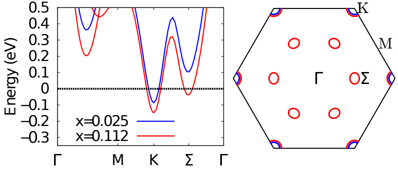

$$\mu^* = \frac{\mu}{1+\mu \ln[\frac{E_F}{\omega_{\log}}]}$$

- for small doping (K occupation) μ^* strongly depends on doping
- at high doping levels (K and Σ occupation) $\mu^* \approx 0.15$ is reasonable
- environmental screening is negligible for high doping levels

⇒ no significant T_c reduction via dielectric screening at optimal doping

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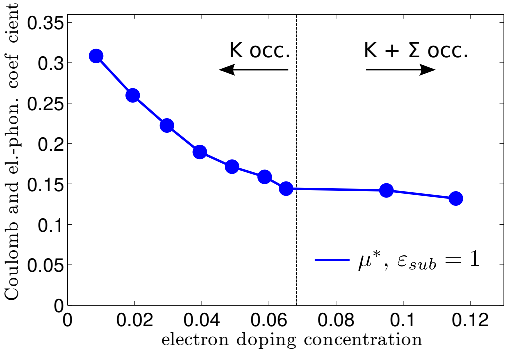

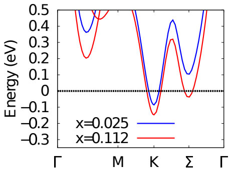

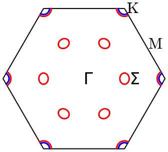

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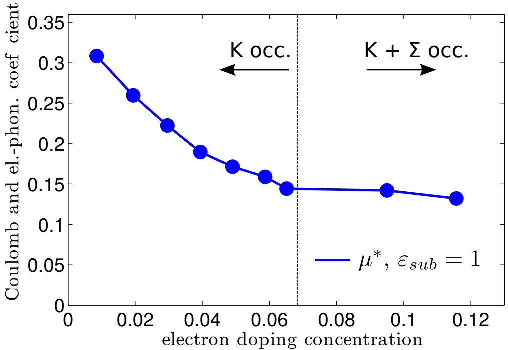

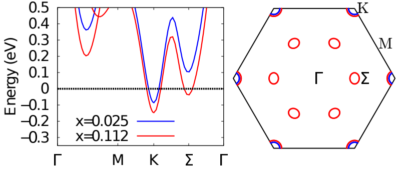

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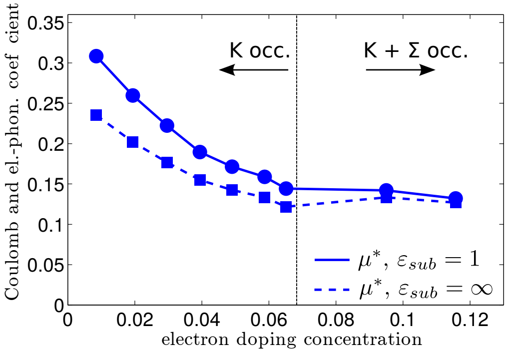

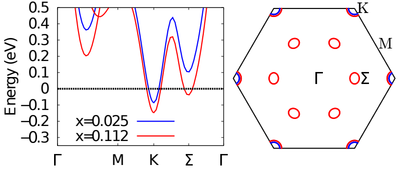

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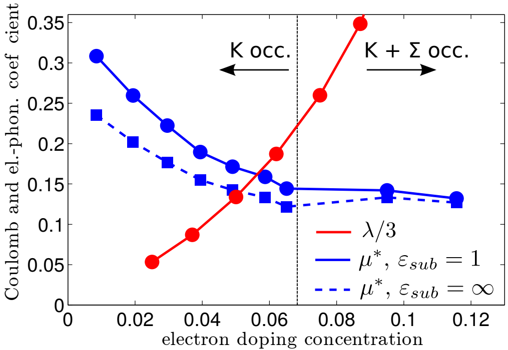

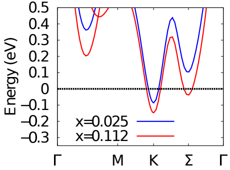

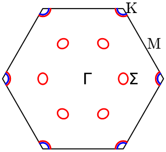

$$T_c = \frac{\hbar\omega_{\log}}{1.2k_B} \exp\left[\frac{-1.04(1+\lambda)}{\lambda(1-0.62\mu^*)-\mu^*}\right]$$

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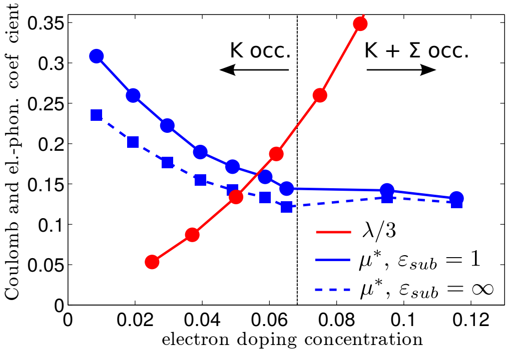

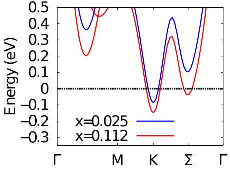

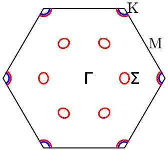

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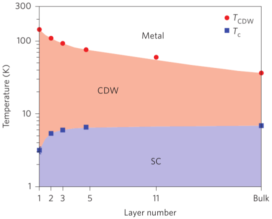

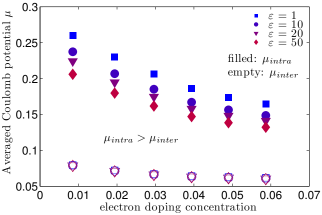

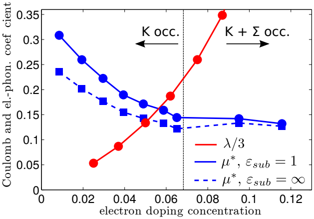

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- there is just a vanishing effect to superconducting properties

⇒ layer dependence of T_c might trace back
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  - enhanced impurity concentrations

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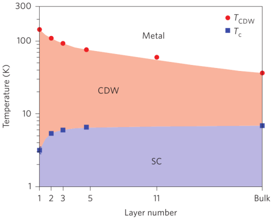

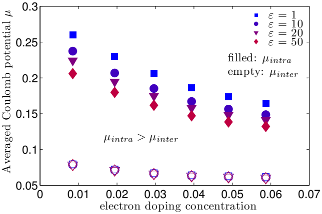

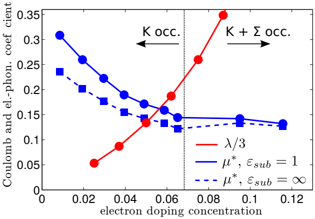

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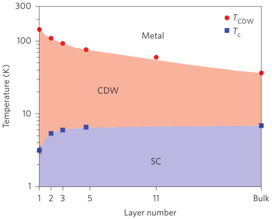

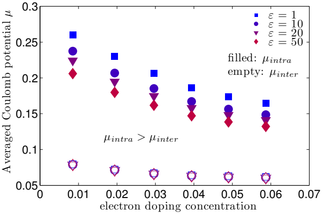

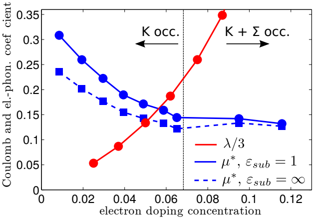

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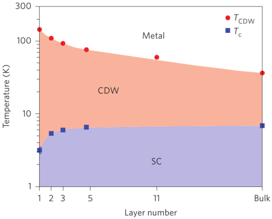

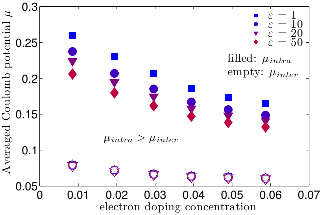

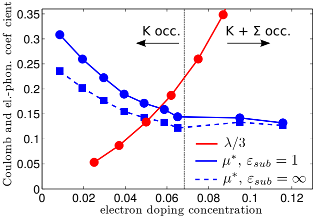

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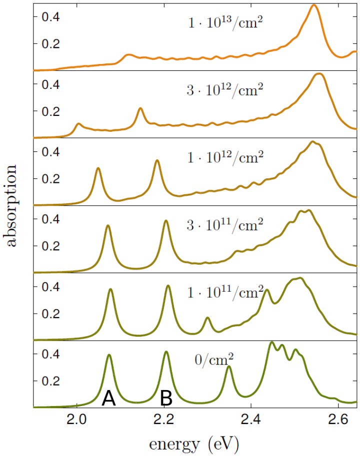
Many-Body Excitations in TMDC Semiconductors



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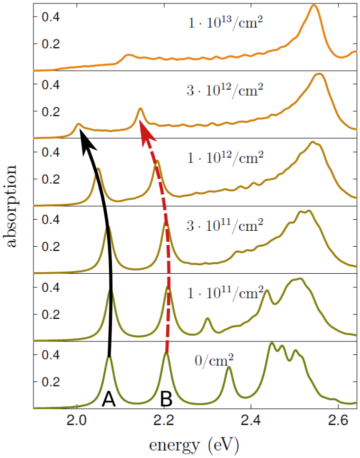

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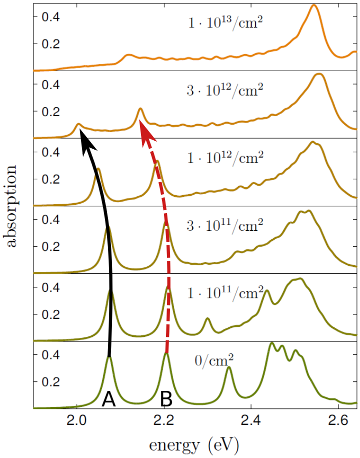
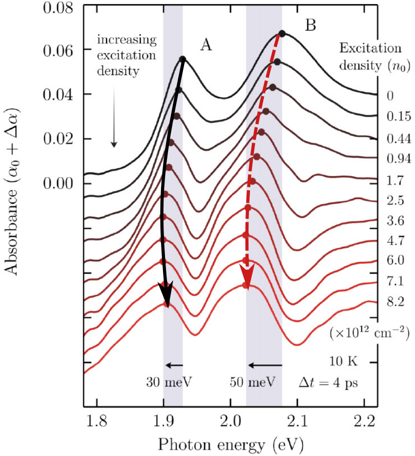
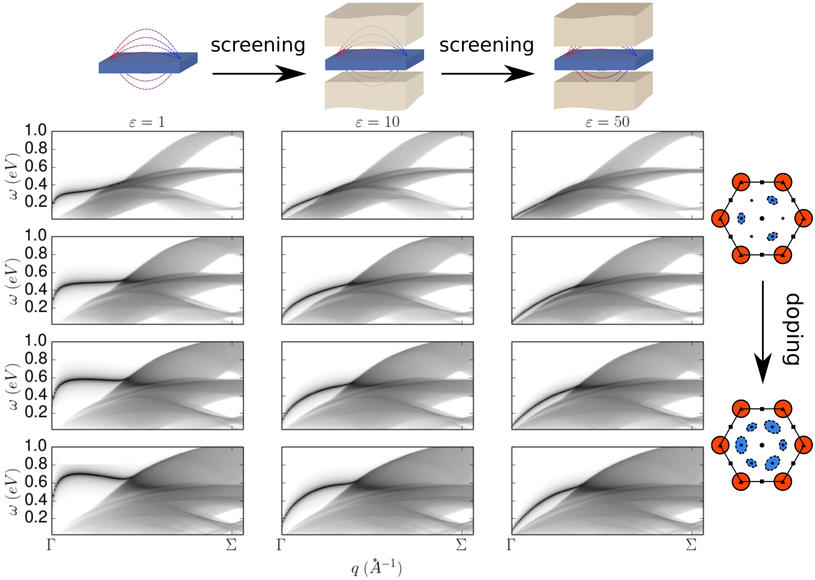




Many-Body Excitations in TMDC Metals



Thank you for your attention!