Quantum Transport Study of Metal-TMD Contacts: Role of the Dielectric Environment

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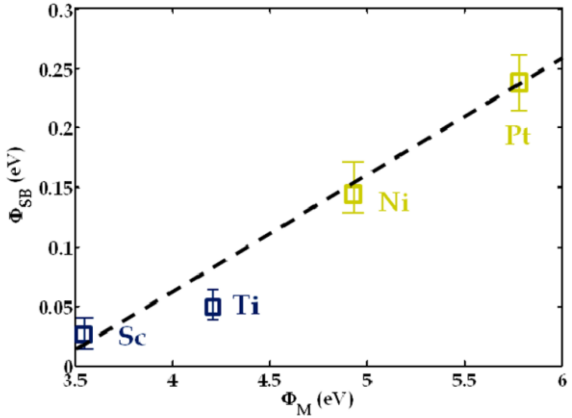
Outline

- Introduction and the PETRA solver
- Simulation methodology
- Results
    - Effect of surrounding dielectric
    - Effect of length of the $\mathrm{low} - \kappa$ dielectric
- Conclusions and Future works

Introduction

- Metal contacted to TMD ➔ high ϕ_B, MIGS ➔ high contact resistance (R_c).

Experimental



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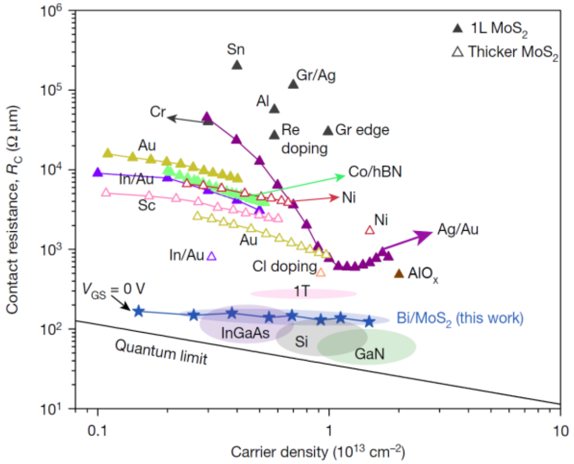
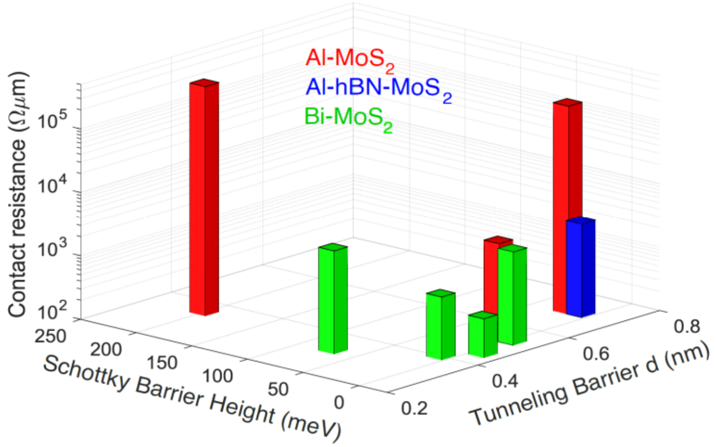
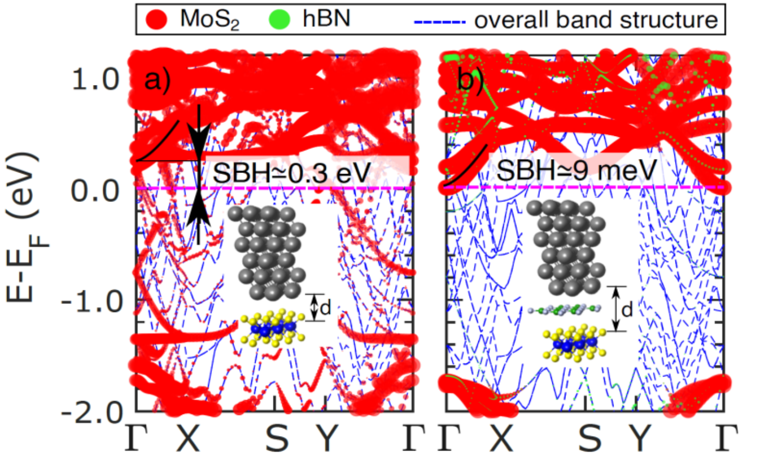
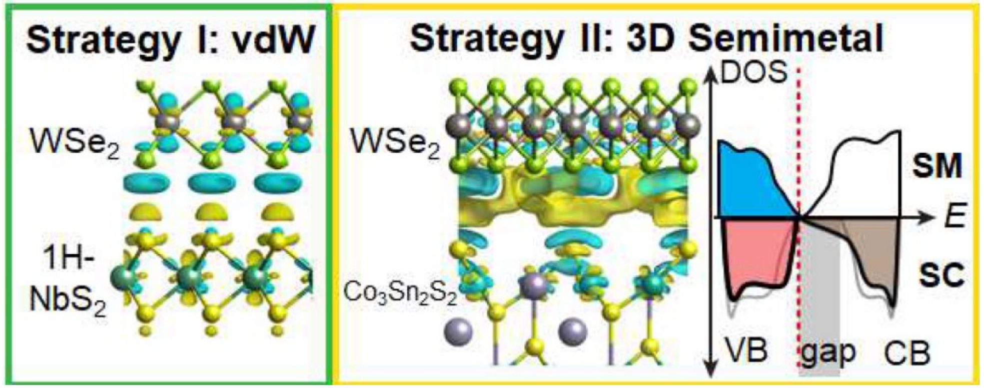


Shen, P.-C. *et al. Nature* **593**, 211–217.





Lizzit, D. et al, IEDM 2022



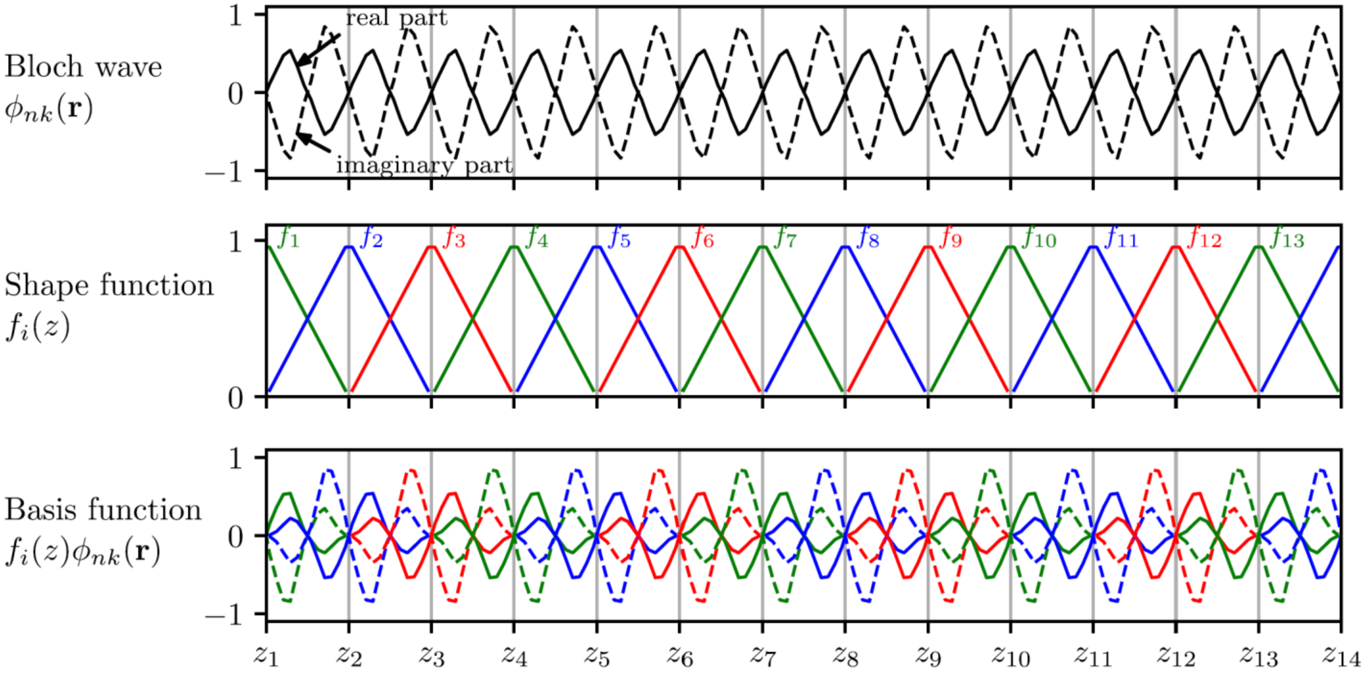
Yang, N. *et al.* IEDM 2022

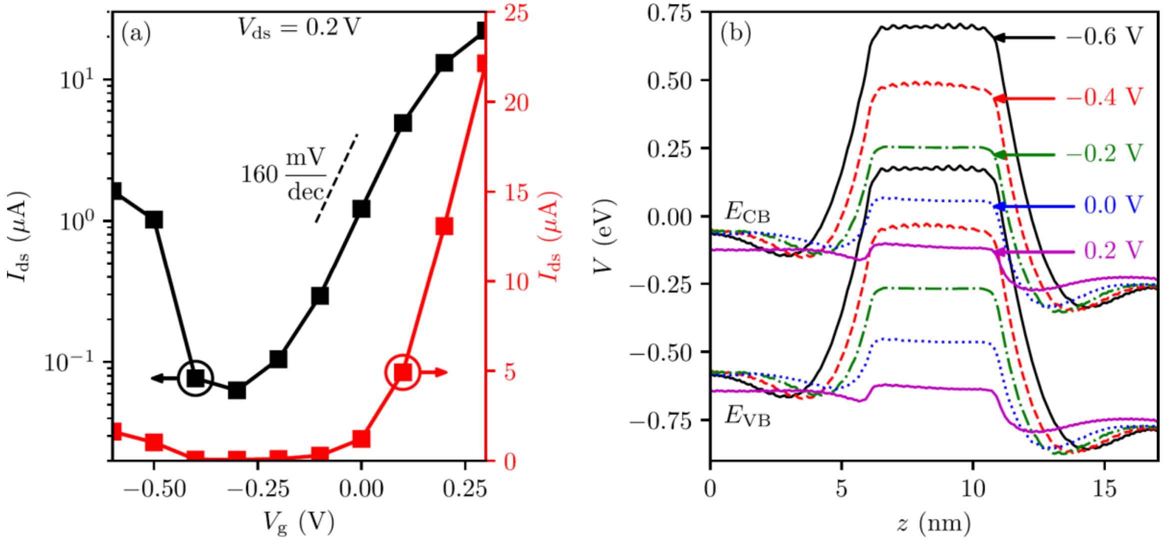
Computational

★ **Our strategy:** Low-κ surrounding dielectric to reduce R_c.

Quantum Transport Using PETRA

Plane-wave Electron TRAnsport (PETRA) ➔ an in-house quantum transport solver [1-2]





Real space ballistic transport of an aGNR using PETRA

Key highlights:

- Atomic and device scales decoupled.
- Bloch wave basis, FEM discretization.
- Computational efficiency using FFT.

1. **Van de Put et al.** Scalable atomistic simulations of quantum electron transport using empirical pseudopotentials. *Computer Physics Communications* **244**, 156–169 (2019).
2. **M. Van de Put**, “Plane-wave Electron TRAnsport.” https://gitlab.com/petra-sim/petra.

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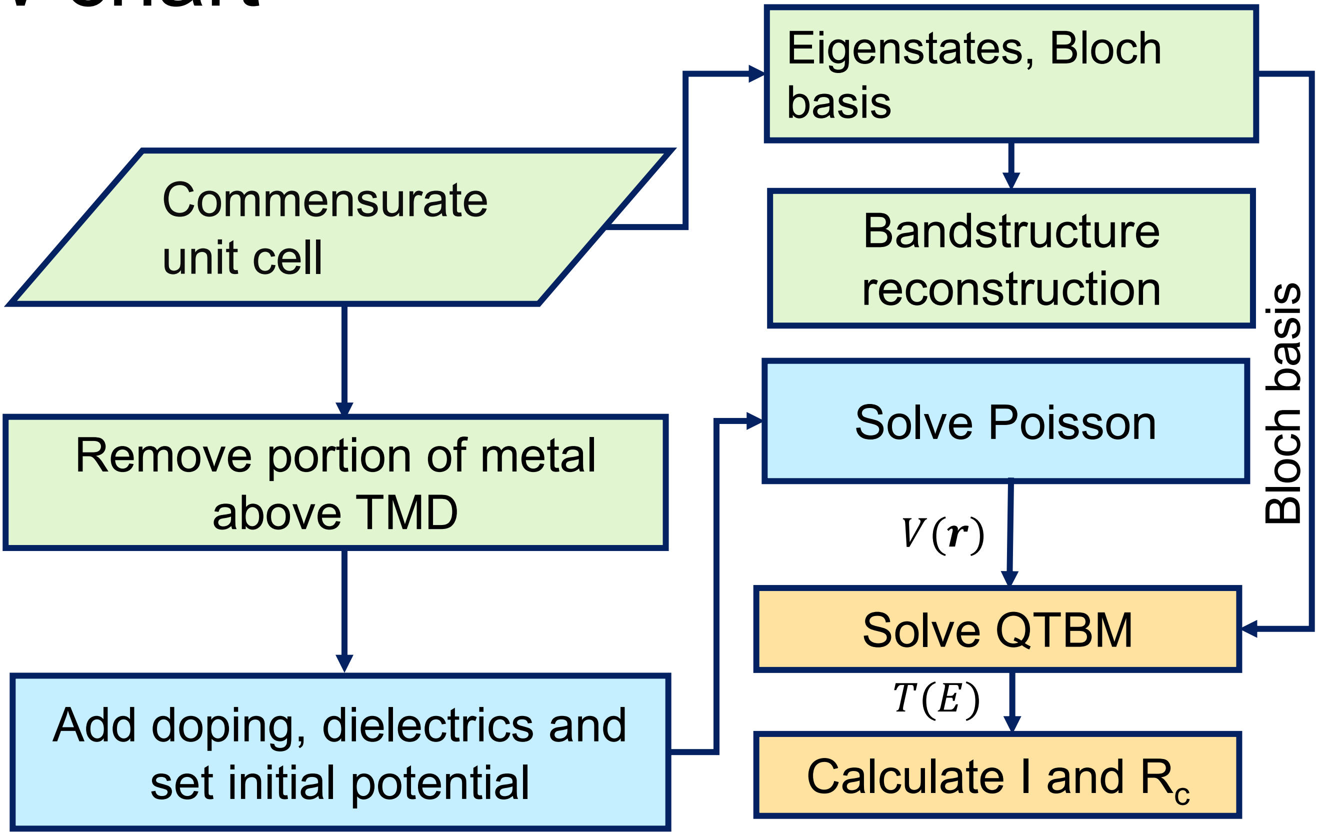
Simulation flow chart



Three steps in our simulation methodology

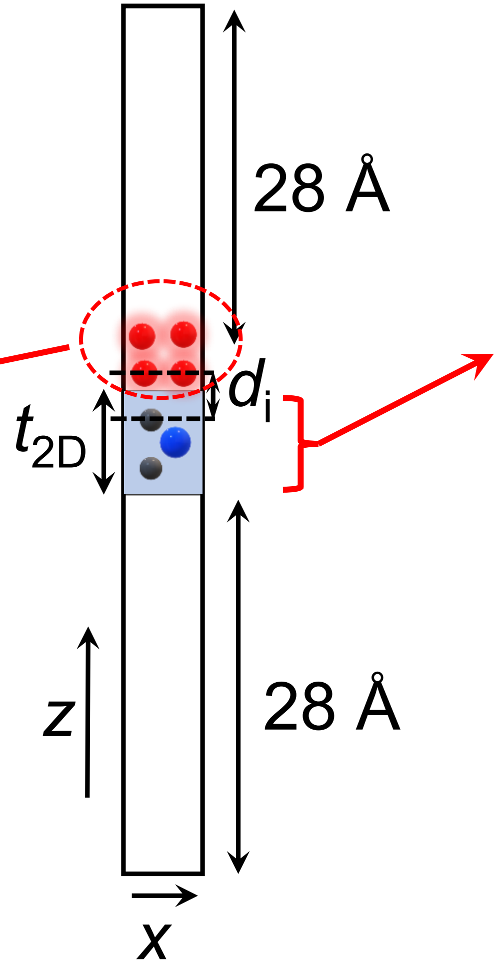
Step 1 : Creating the contact heterostructure.

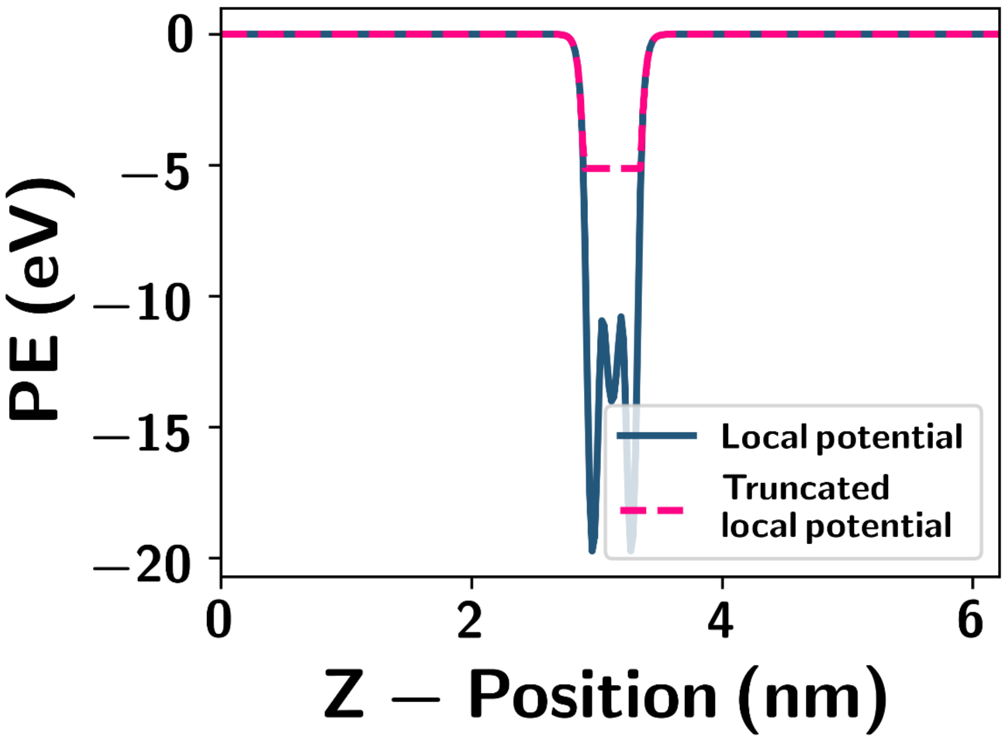
Step 2 : Add doping, dielectrics and solve Poisson.

Step 3 : Solve QTBM, extract T(E), and calculate R_c.

Materials modeling

Metal atoms ➔ empirical pseudopotentials, $E_{\text{cut}} = 250\ \text{eV}$

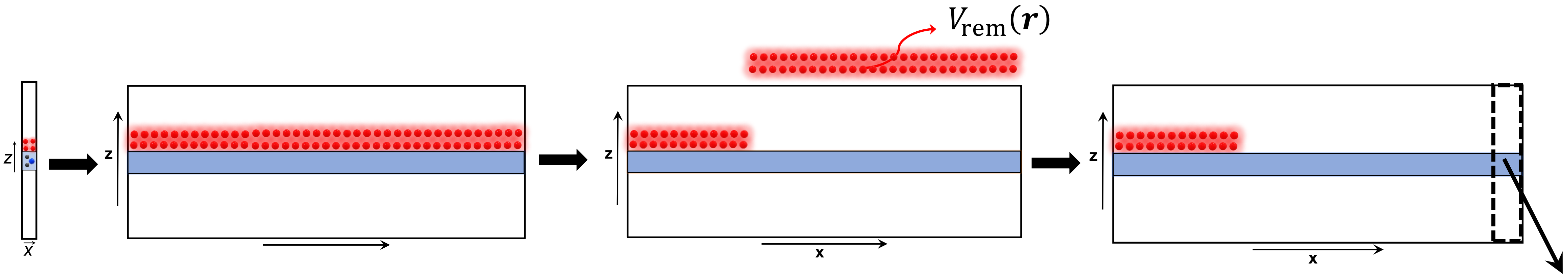




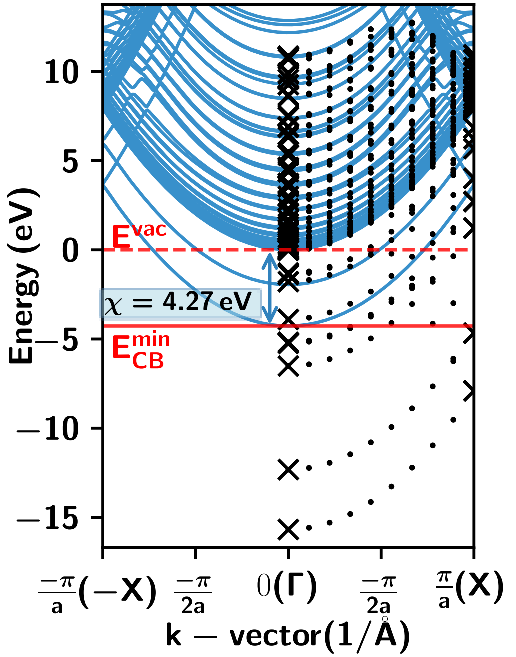
- Local potential from VASP ➔ $x - y$ averaged and truncated at $E_{\text{trun}}^{\text{loc}} (= -5.13\ \text{eV})$
- Solve the single particle Schrödinger equation for the unit cell

$$\frac{-\hbar^2}{2}\nabla.\left[m_{\text{eff}}^{-1}(\boldsymbol{r})\cdot\nabla u_{nk}(\boldsymbol{r})\right] + \left[V_{\text{m}}(\boldsymbol{r}) + V_{\text{TMD}}(\boldsymbol{r})\right]u_{nk}(\boldsymbol{r}) = E_{nk}u_{nk}(\boldsymbol{r})$$

Creating the contact heterostructure

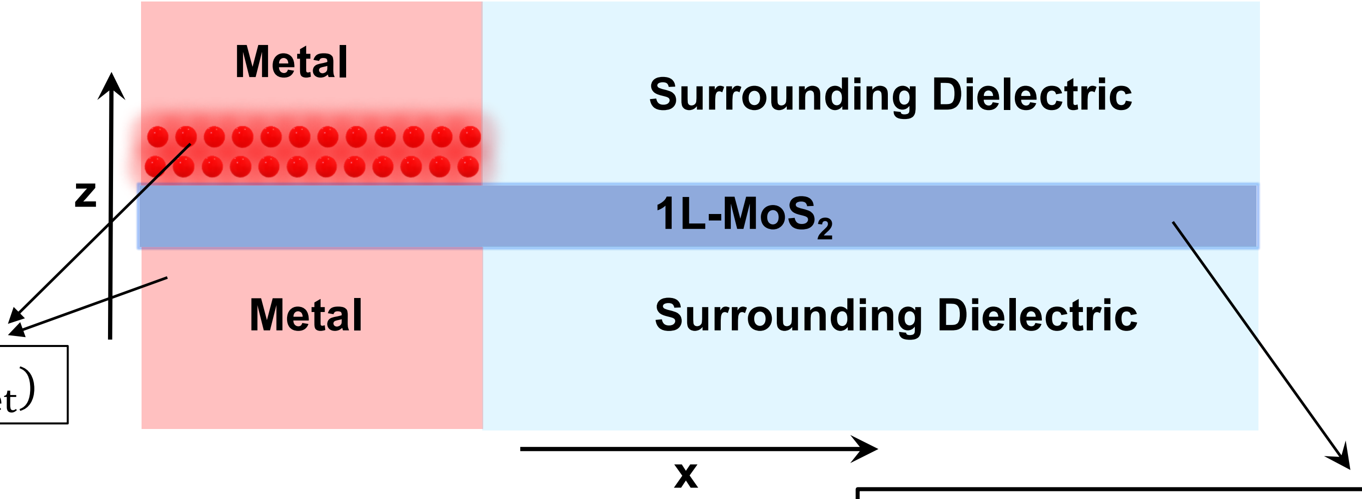


Unit cell ➔ Repeat periodically along x ➔ Eliminate portion above TMD



Reconstructed bandstructure using Bloch wave basis

R_c calculation



from VASP

$$\rho_{\mathrm{met}}(\boldsymbol{r}) = DOS_{\mathrm{met}} \cdot (V(\boldsymbol{r}) - \phi_{\mathrm{met}})$$

$$\rho_{\mathrm{TMD}}(\boldsymbol{r}) = \frac{m^* k_{\mathrm{B}} T}{t_{\mathrm{2D}} \pi \hbar^2} ln\left(1 + e^{-\left(\frac{V(\boldsymbol{r}) - \chi_{\mathrm{TMD}} - E_{\mathrm{F}}}{k_{\mathrm{B}} T}\right)}\right)$$

Poisson:
- Appropriate dielectric tensors for different regions.
- 1L-MoS$_2$ is *n*-doped to $N_{\mathrm{2D}} = 1 \times 10^{13} \mathrm{cm}^{-2}$
- All boundaries ➔ Neumann BC and Top right corner ➔ Dirichlet BC (point).

Schrödinger:
- 0.1 V bias to right edge of simulation domain.
- Device Hamiltonian ➔ wavefunctions (QTBM) ➔ T(E, k_y).
- $I = \frac{2q}{h} \int \mathrm{d}k_y \int \mathrm{d}E\, T(E, k_y)\big(f_L(E, \mu_L) - f_R(E, \mu_R)\big)$ and R_c from Ohm's law.

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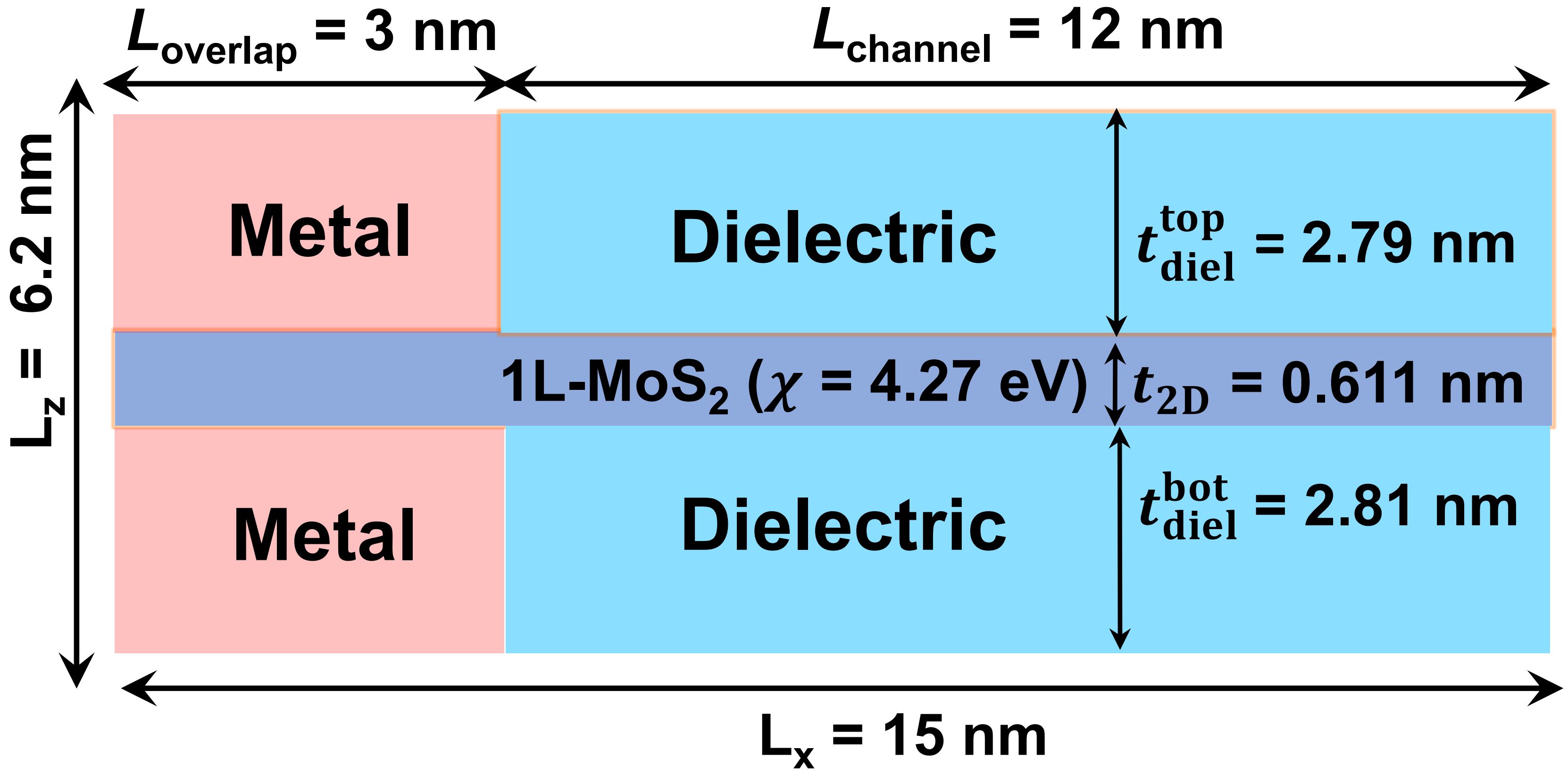
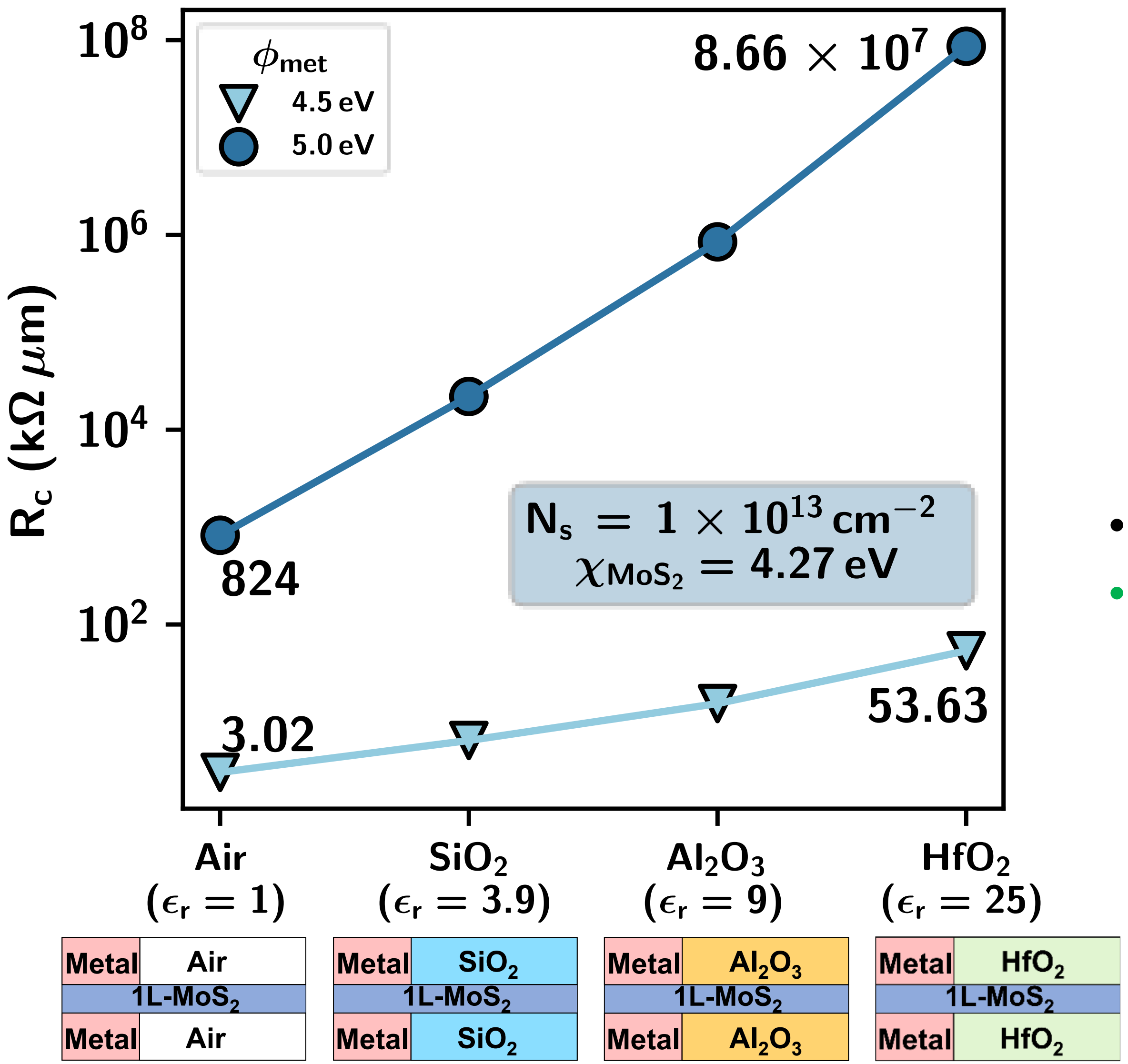
Contact setup



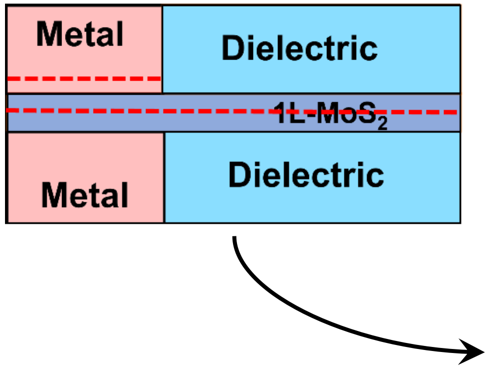
- 1L-MoS$_2$ is n-doped to $N_s = 1 \times 10^{13}\ \text{cm}^{-2}$.
- Four surrounding dielectrics ➔ Air, SiO$_2$, Al$_2$O$_3$ and HfO$_2$.
- Uniform effective mass tensor (corresponding to MoS$_2$) across the entire simulation domain.

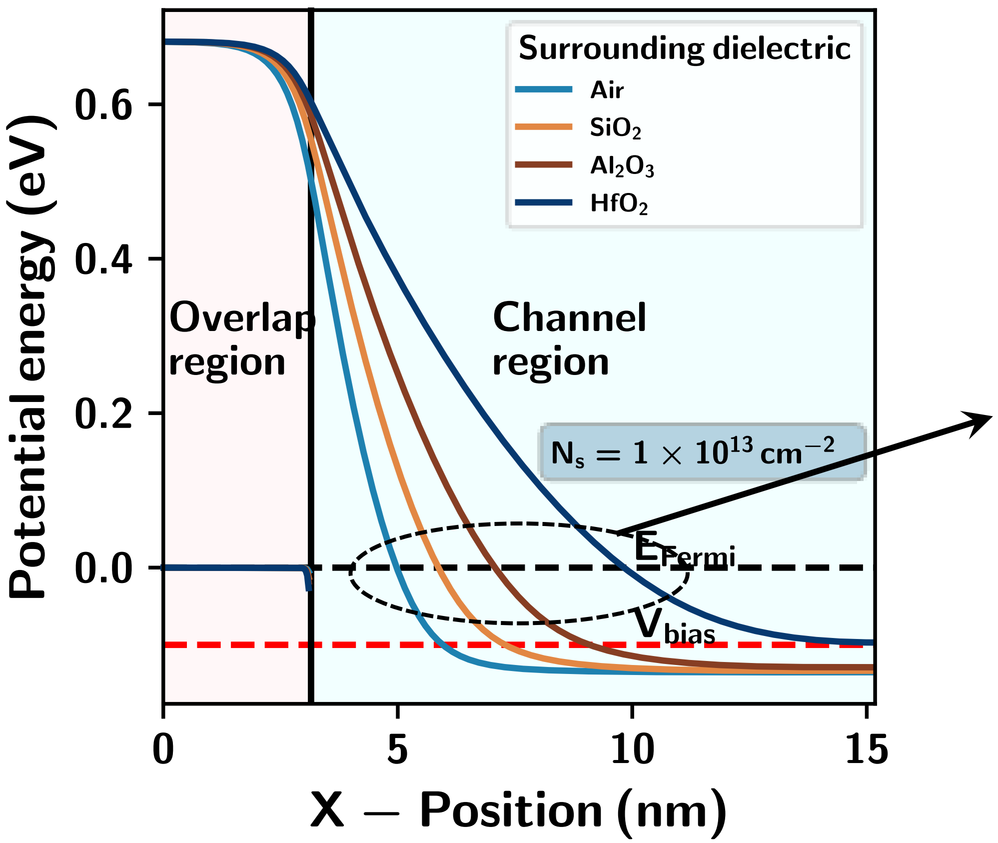
Results - Effect of surrounding dielectric

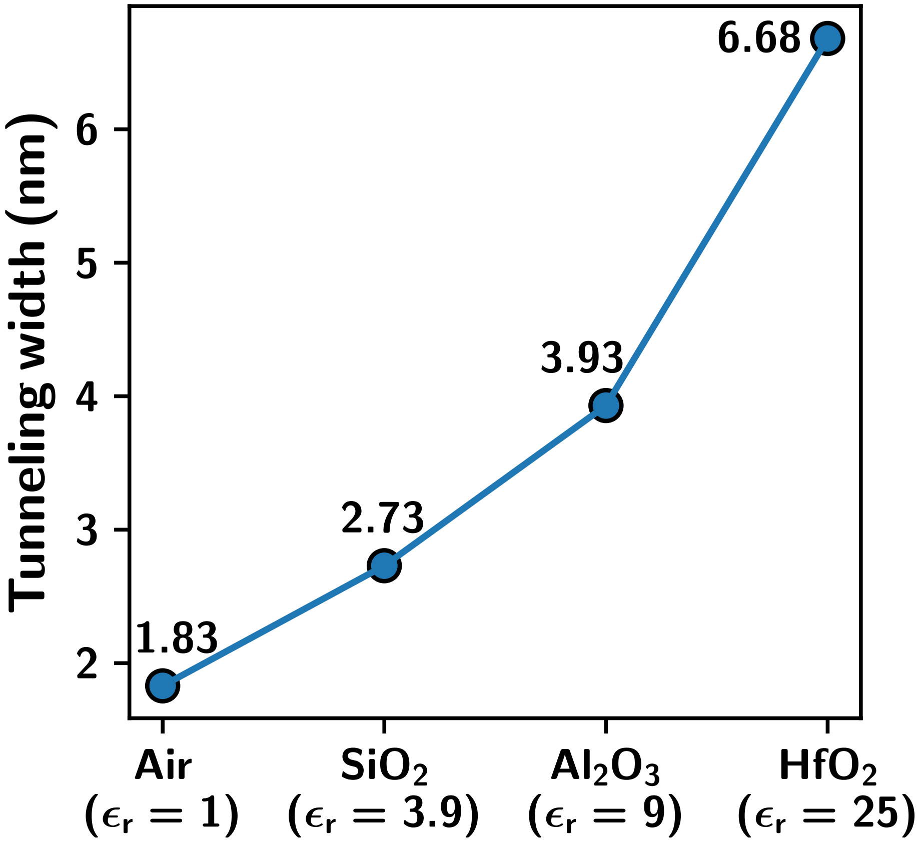


- ϵ_r of surrounding dielectric ↑ ➔ R_c of the contact ↑
- Low-κ surrounding dielectric ➔ lower R_c

Results - Effect of surrounding dielectric

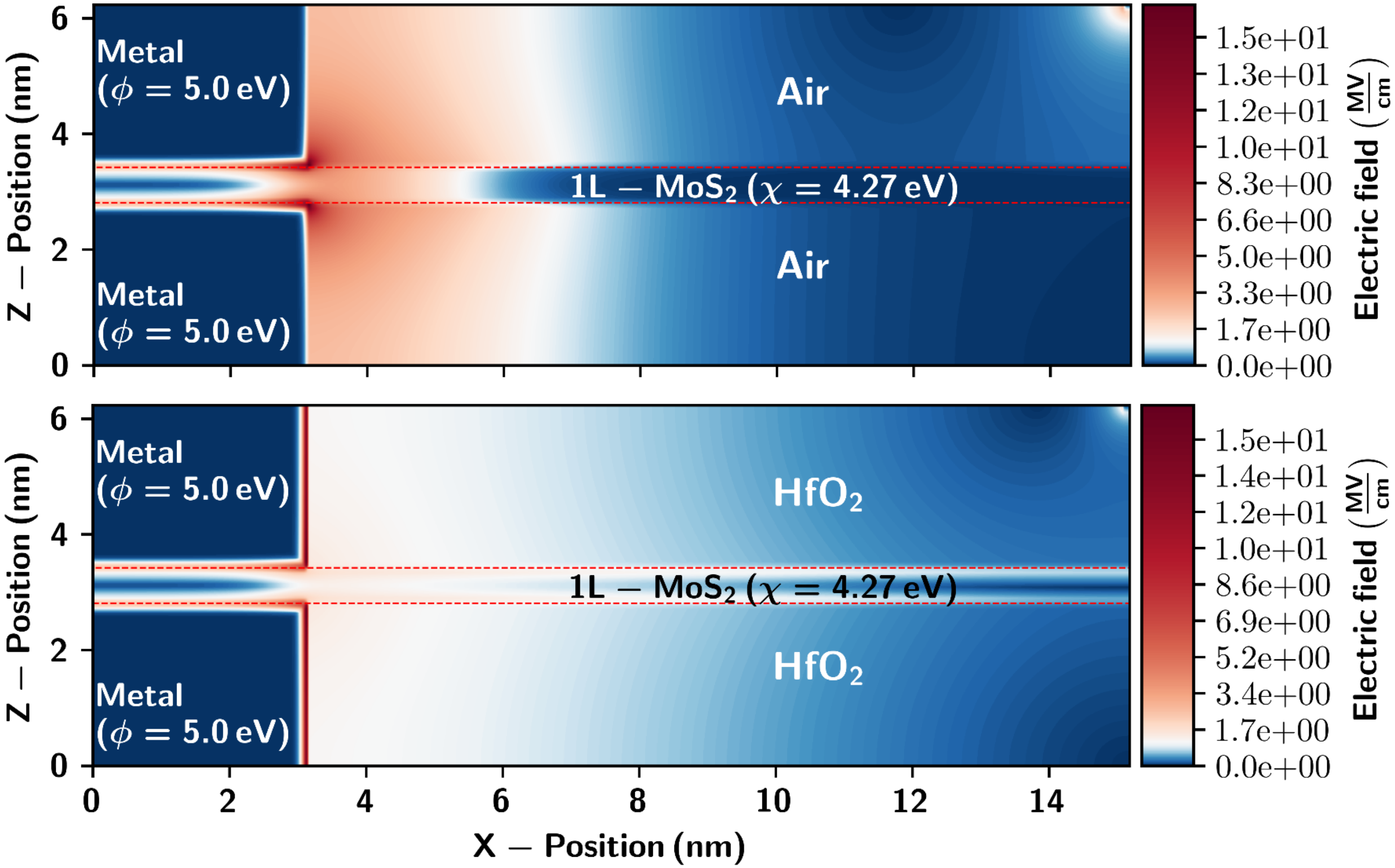






- ϵ_r of surrounding dielectric ↑ ➔ Tunneling width for electrons ↑
- ϵ_r ↑ from 1 to 25 ➔ 3.65x increase in tunneling width.

Results - Electric field profile



High-κ surrounding dielectric ➔ dielectric screening ↑ ➔ depletion and tunneling widths ↑ ➔ R_c ↑

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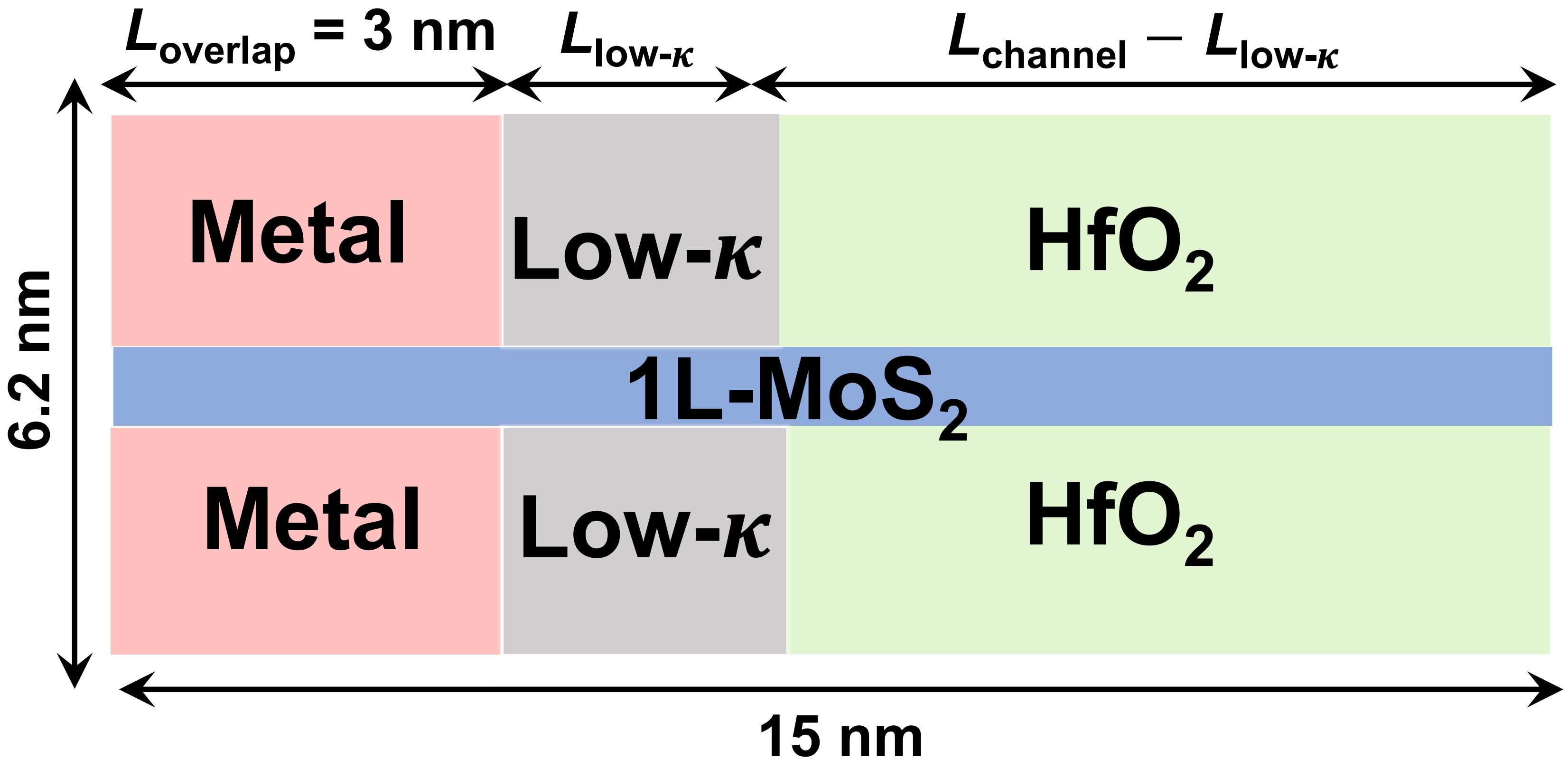
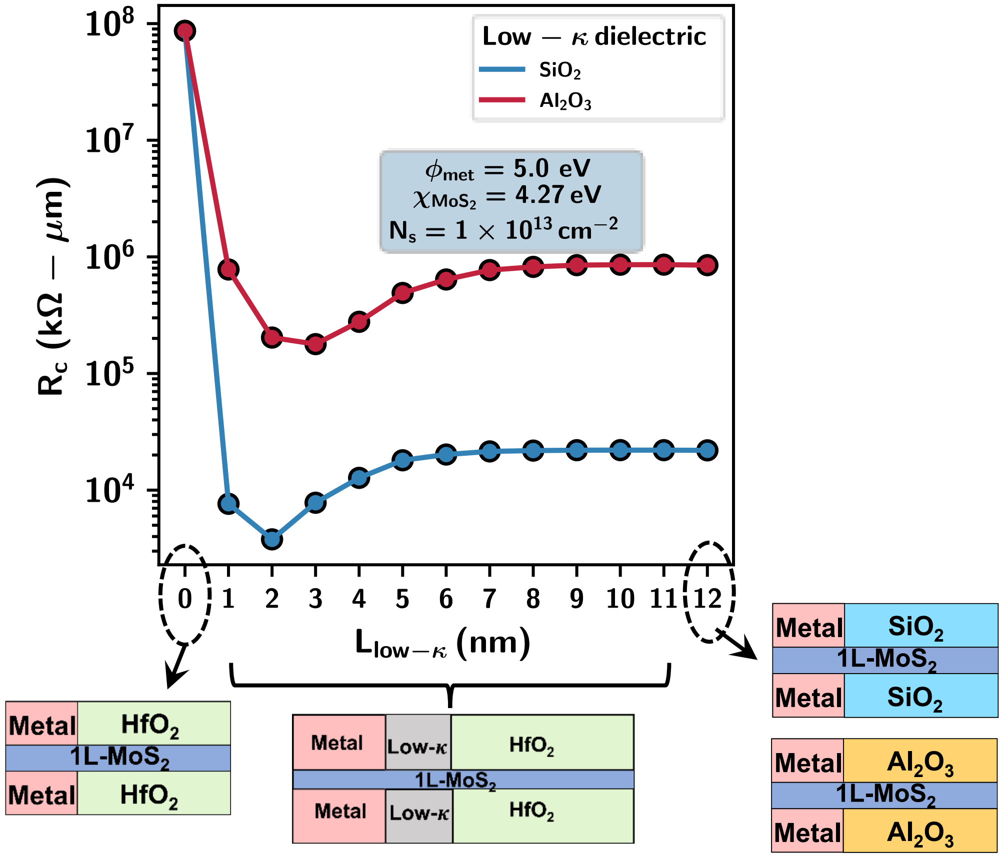
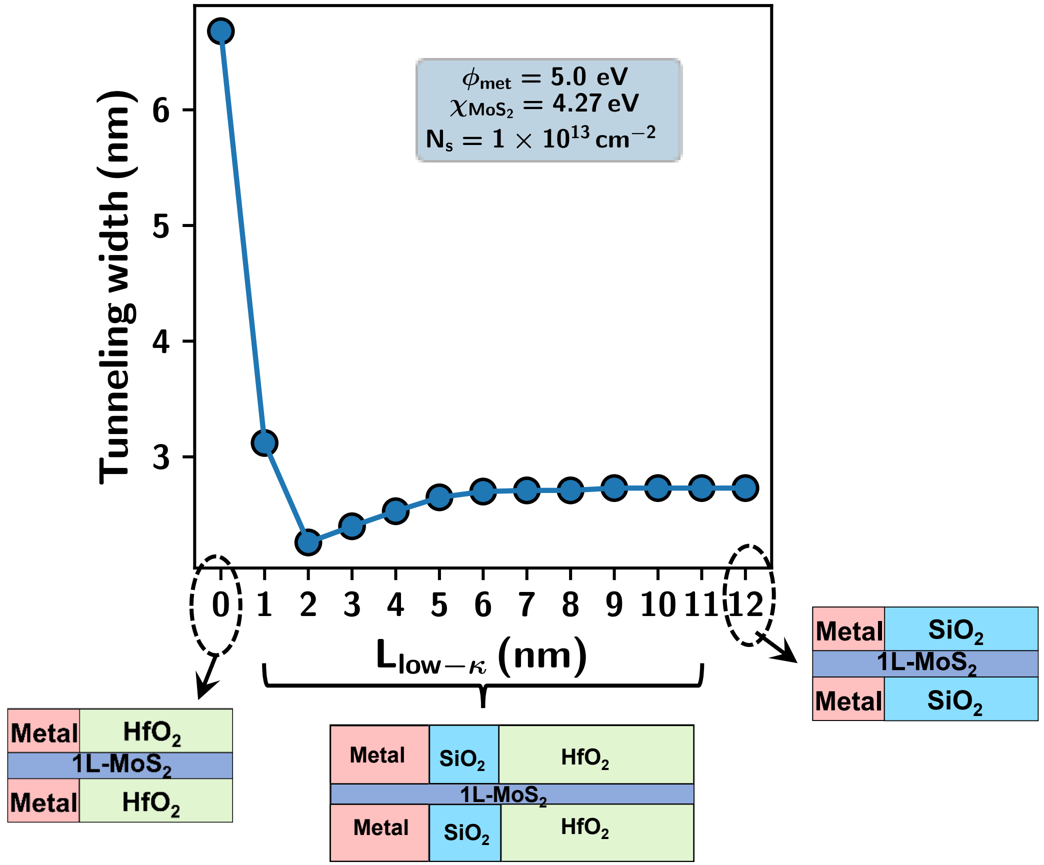
Effect of $L_{\mathrm{low}-\kappa}$



- Vary $L_{\mathrm{low}-\kappa}$ (from 0 nm to 12 nm) to investigate its impact on R_c.
- All other parameters are same as the previous simulations.

Effect of $L_{\mathrm{low}-\kappa}$





- 2nm of SiO_2 at the edge of metal ➔ 3x ↓ in tunneling width and ~4 orders ↓ in R_c.
- Advantages : (a) As spacer to isolate S/D from gate. (b) High-κ around the rest of channel ➔ ↑ μ of MoS_2 [1]

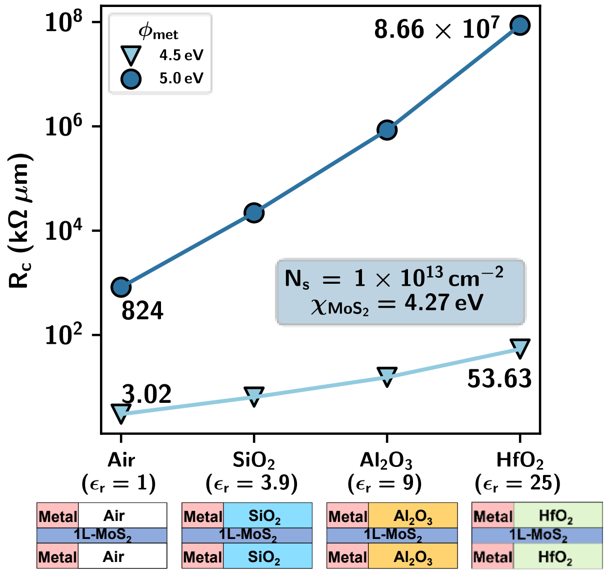
[1] **Ong, Z.-Y** et al. Mobility enhancement and temperature dependence in top-gated single-layer MoS_2. *Phys. Rev. B* **88**, 165316 (2013).

Key conclusions

- Low-κ surrounding environment ➔ weaker screening of fringing field ➔ smaller depletion and tunneling widths ➔ Lower contact resistances.

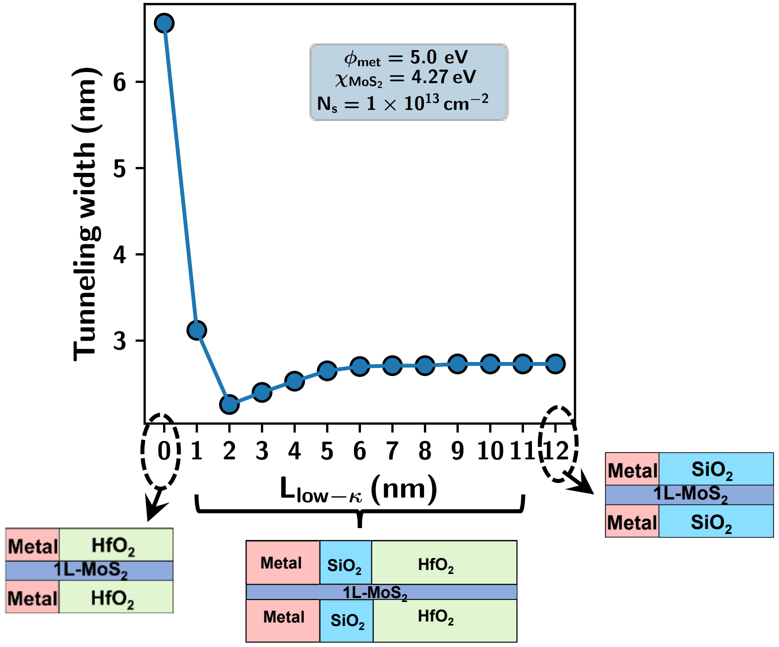
Low-κ surrounding dielectric around monolayer TMDs reduce R_c

- A small layer of Low-κ near the edge of metal is sufficient to reduce R_c by several orders of magnitude.



Future works

- Incorporating Image Force Barrier Lowering (IFBL) into our simulations ➔ reduces R_c values reported in this study, especially for low-κ environments.



Thank you !

Questions ?