Ab-initio enabled TMD calculations

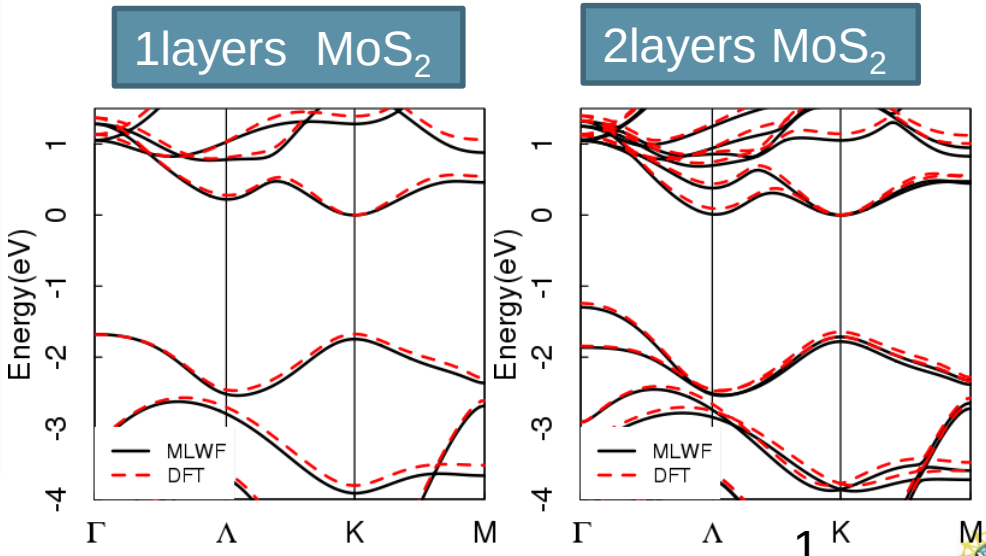
Problem:
- Shortcoming of tight binding(TB): non-transferable parameter sets
- Shortcoming of DFT: High numerical load

Objective:
- Numerically efficient support of Ab-initio representation in NEMO5

Approach:
- VASP and Wannier90: Hamiltonian in Maximally Localized Wannier Functions(MLWF)
- Hamiltonian and MLWF input to NEMO5

$$|\mathbf{R}n\rangle = \frac{V}{(2\pi)^3}\int_{BZ}\sum_{m=1}^{N} U_{mn}^{(\mathbf{k})}\,|\psi_{m\mathbf{k}}\rangle\, e^{-i\mathbf{k}\cdot\mathbf{R}}\, d\mathbf{k}$$

Result/Impact:
- Agreement of NEMO5 dispersion with DFT
- Numerical load comparable to regular TB
- MLWF basis compatible with all NEMO5 transport features (e.g. scattered quantum transport)



Poisson with Subatomic resolution

Problem:

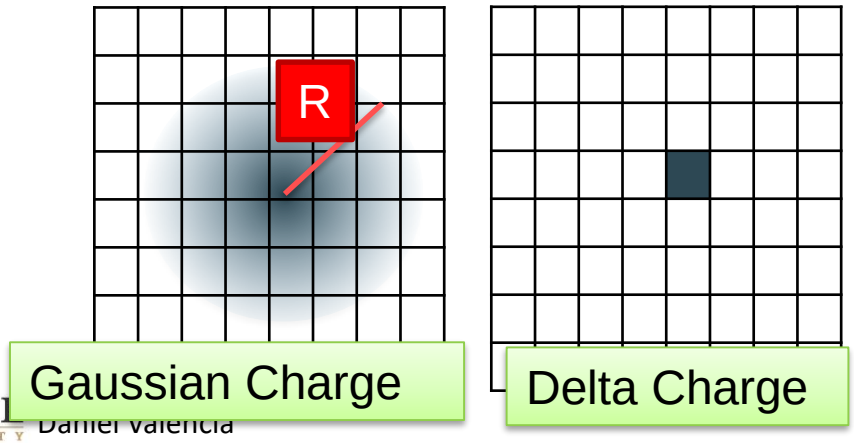
- Low dimension simulation requires higher spatial resolution
- Delta charge distribution on the FEM cell becomes unphysical and can cause numerical divergence

Objective:

- Gaussian charge distribution among FEM cell

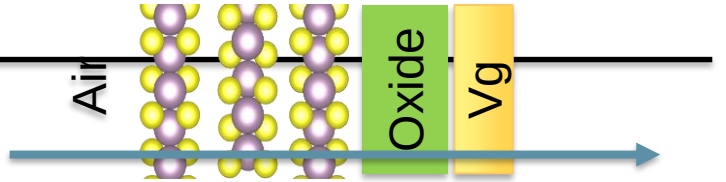
Approach:

- Charge distributed among neighboring FEM cells



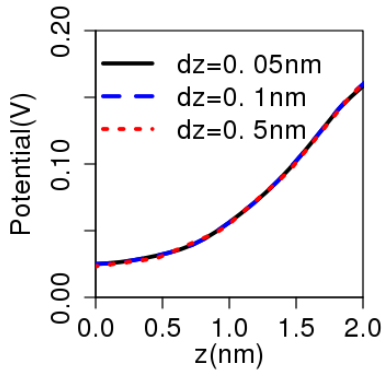
Result/Impact:

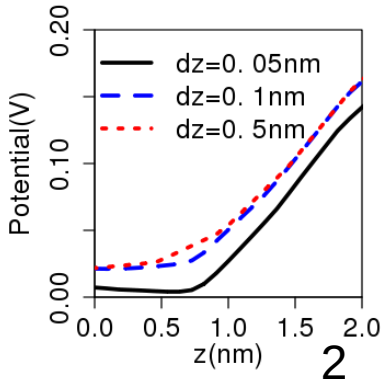
- Mesh refinement is possible without divergence
- Resolution of charge, potential in the atomic scale



Gaussian Charge

Delta Charge





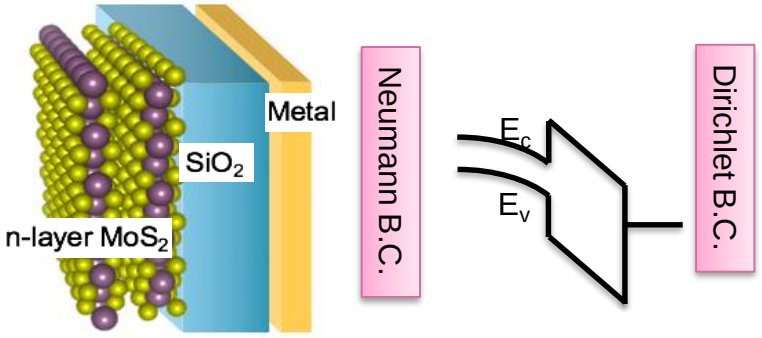
MoS_2 Metal-oxide-Semiconductor

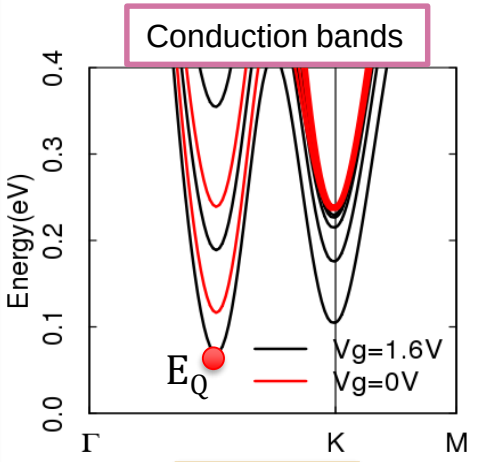
Problem:
- How does gate voltage affect the 2D material?

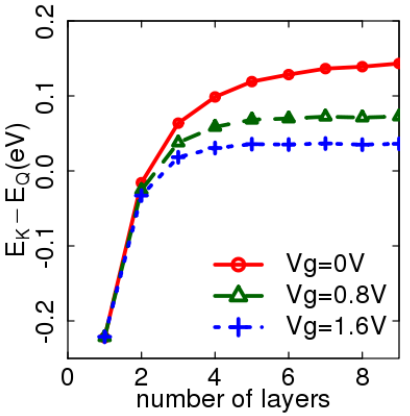
Objective:
- Study the band structure change under the gate voltage.

Result/Impact:
- DFT–equivalent, but efficient Hamiltonian used to accurately describe MoS2 devices
- Band offsets are function of gate voltages and layer thickness
- Valley wave functions differ significantly in their spatial distribution
- Different gate response of the 2 conduction band valleys. This can serve for switching device applications

Approach:
- Schrodinger-Poisson solved.
- Wannier function basis is used for device Hamiltonian.







5 layer

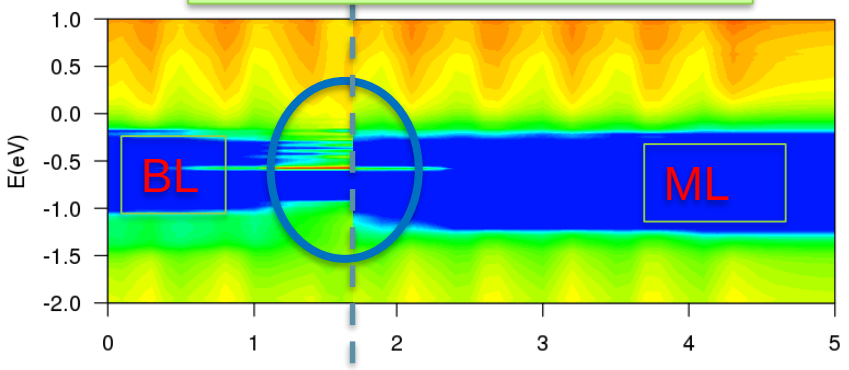
ML/BL Surface states

- Importance: ML/BL common structure in vertical TMD structure

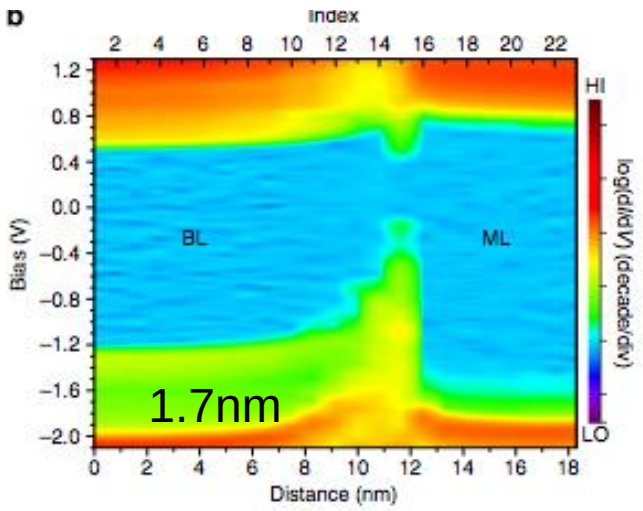
Methodolgy:
- DFT relaxation of interface
- Sc-born scattering to probe density of states
- Including acoustic and optical phonon scattering
- Charge self-consistent calculation

Impact:
- Identify energy favored interface. (S ending, Mo ending)
- Identify QW depth
- Study the influence on current flow w/wo interface state

NEMO preliminary result



1.7nm



[1] C. Zhang, etc, *Nat. Commun.*, vol. 6, p. 1–6, 2016.