Spin-valley transport in magnetic 2D materials through multiscale simulations

Damiano Marian[1,2], David Soriano[3], Prabhat K. Dubey[1], Emmanuele Cannavò[1], Enrique G. Marin[4], Gianluca Fiori[1]

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[2]Dipartimento di Fisica, Università di Pisa (Italy)
[3]Departamento de Física Aplicada, Universidad de Alicante (Spain)
[4]Departmento de Electrónica, Universidad de Granada (Spain)

IWCN - 13th June 2023

Outline

- **Motivations**
- **Multiscale approach**
- **Spin-valve transistor based on bilayer CrI_3**
  - Bilayer CrI_3
  - Spin filter and Spin-valve transistor
- **Valley-spin transport in $CrBr_3/WSe_2/CrBr_3$ vdW heterostructure**
  - Proof-of-concept valleytronic FET
  - $CrBr_3/WSe_2/CrBr_3$ vdW HS and valley transport

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Motivations

2D magnetic materials – advantages over 3D counterpart:

- They can be easily interfaced with other 2D materials
- They present stacking-dependent magnetic properties
- Their ground state magnetization can be modified with electric fields

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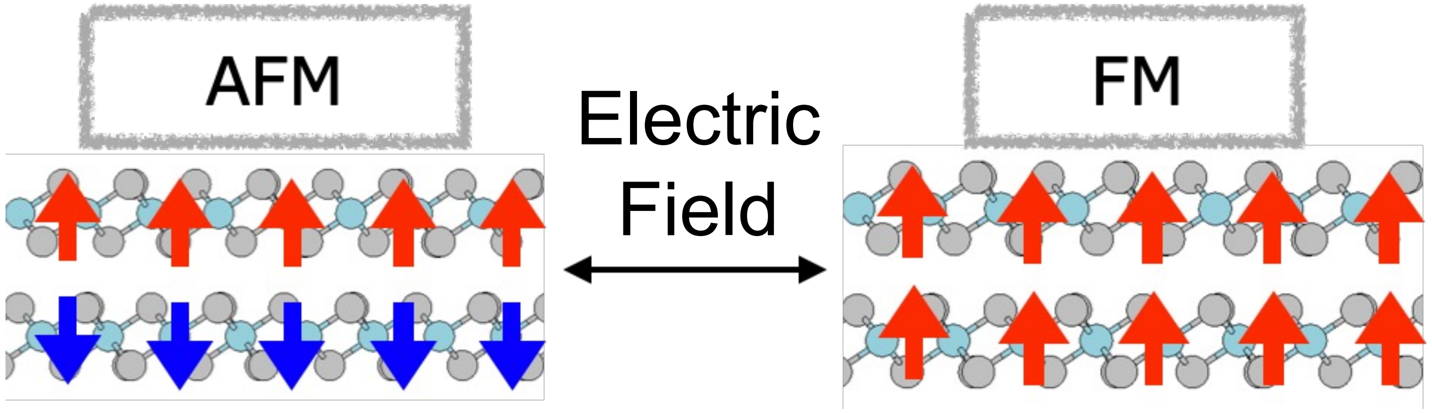
Experimentally and theoretically it has been observed that the electric field can control the interlayer magnetism



* Jiang et al., Nature Nanotechnology, 13, 549 (2018)

* Jiang et al., Nature Materials, 17, 406 (2018)

* Huang et al., Nature Nanotechnology, 13, 544 (2019)

Search for spin/valley device concept fully electrically controlled

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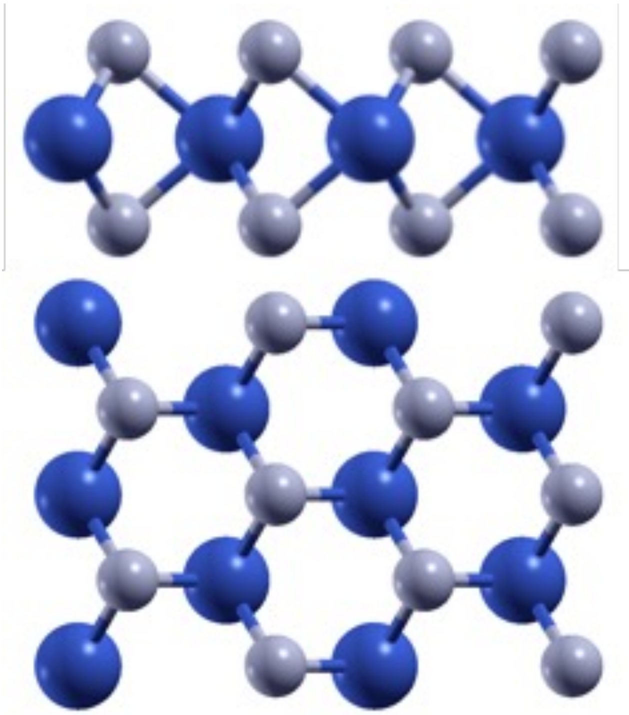
Multiscale approach

1

Ab-initio DFT

Electronic properties



Quantum Espresso

P. Giannozzi et al. J. Phys.: Cond Matt., 21, 395502 (2009)

D. Marian, et al., J. Comp. Elect. 2023

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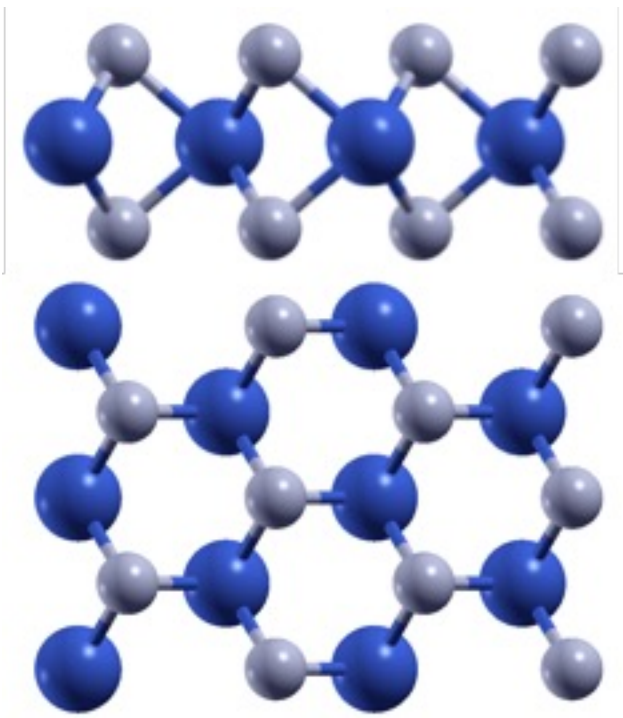

Quantum Espresso

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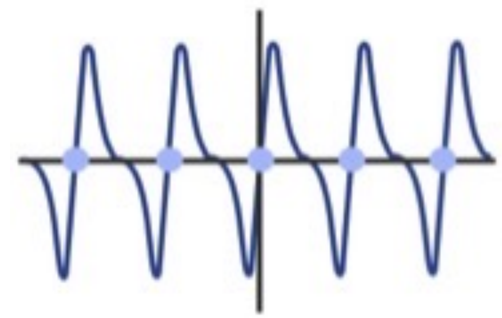
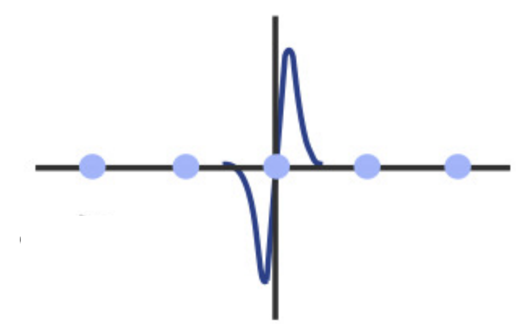
2

Wannier (MLWF)



TB-*like* Hamiltonian



Wannier90

N. Marzari et al Rev. Mod. Phys., 84, 1419 (2012)

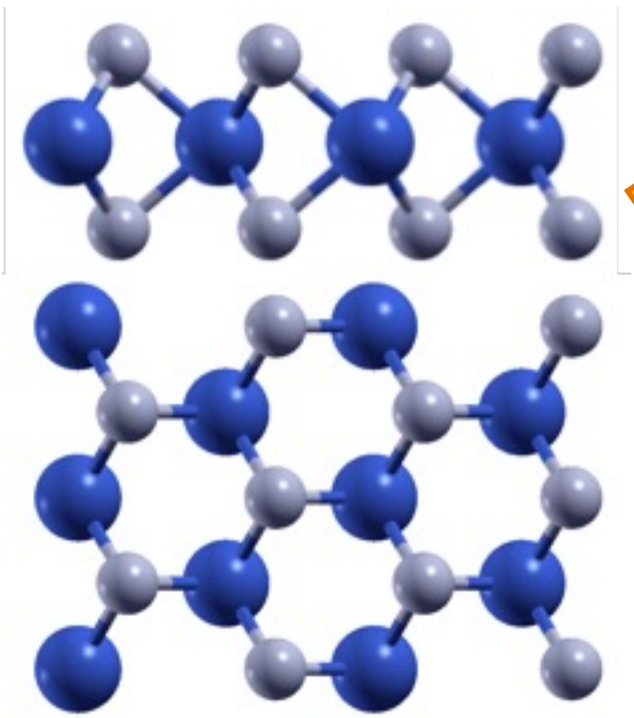
D. Marian, et al., J. Comp. Elect. 2023

Multiscale approach

1

Ab-initio DFT

<u>Electronic properties</u>



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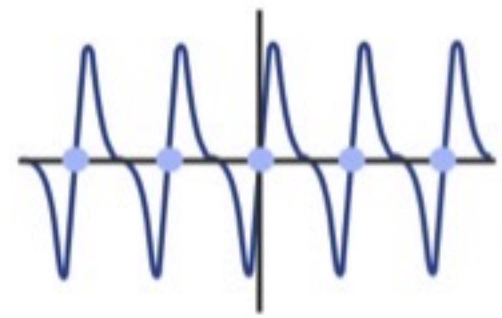

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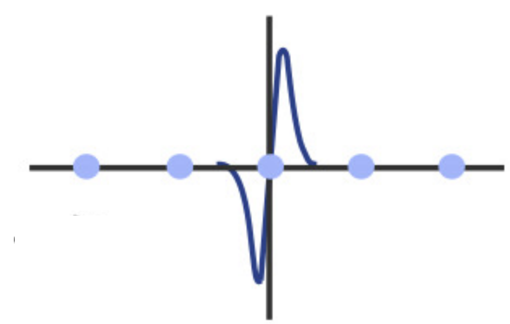

Wannier90

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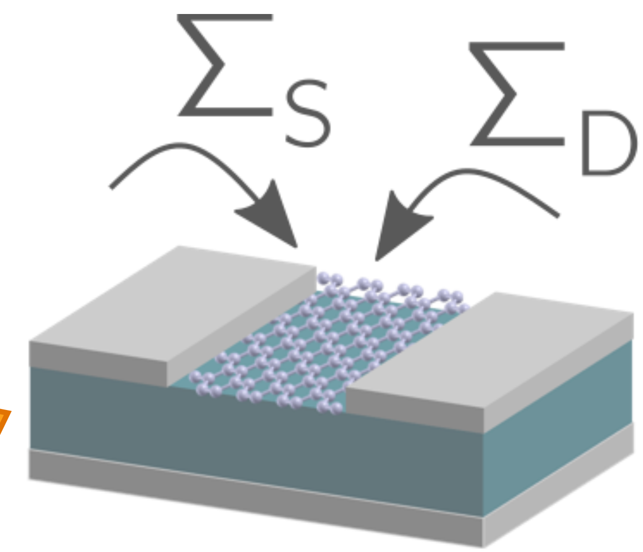
3

<u>Transport</u>

NEGF

Self-consistent

Possion Equation



NanoTCAD-ViDES

http://vides.nanotcad.com/vides/

D. Marian, et al., J. Comp. Elect. 2023

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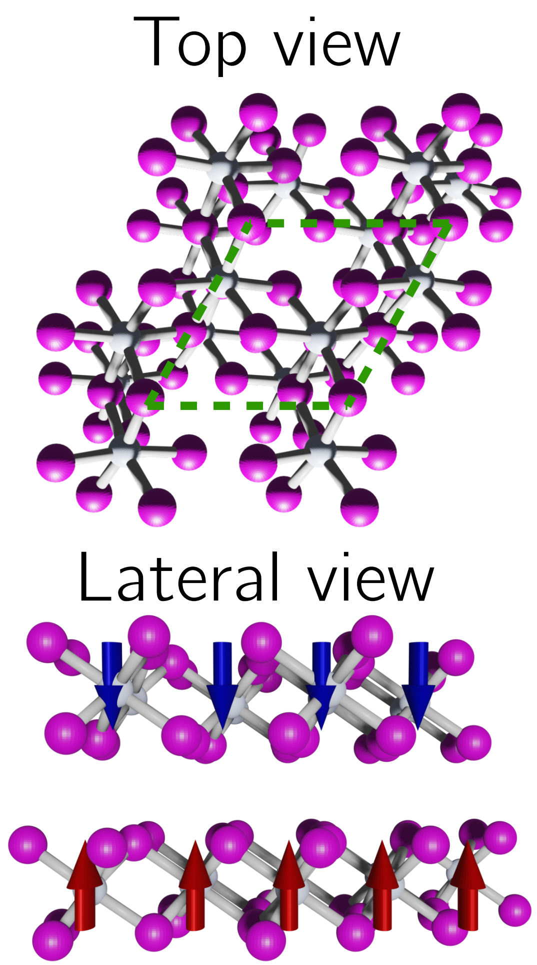
Bilayer CrI_3: electronic and magnetic properties

CrI_3 bilayer in monoclinic stacking: antiferromagnetic (AFM) ground state



N. Sivadas et al. Nano Letters, 18, (2018)

D. Soriano et al. Solid State Comm., 299, 113662 (2019)

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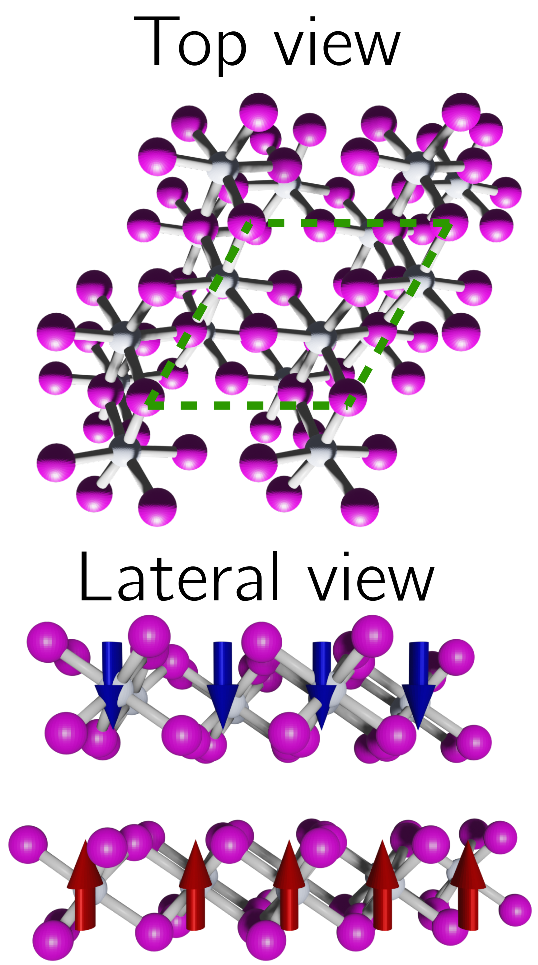

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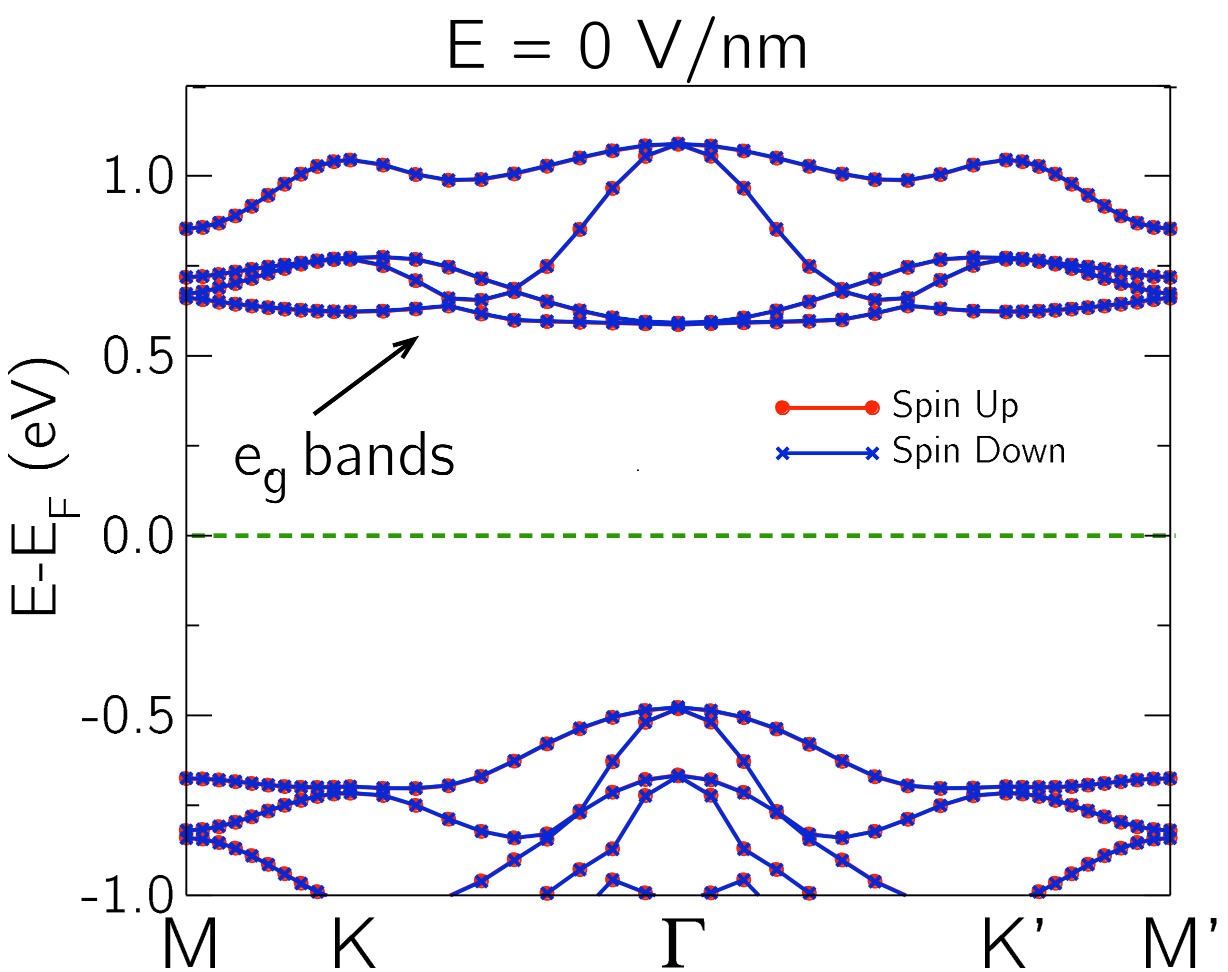
Band structure of bilayer CrI_3

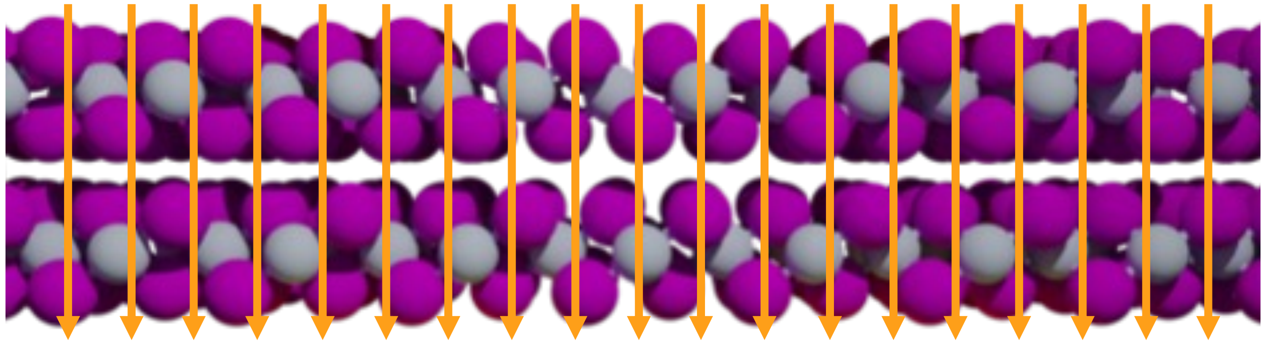


D. Marian et al. NPJ 2D Mater. Appl. (2023)

Bilayer CrI_3 under external electric field

What happens if we apply a vertical electric field?

Electric field



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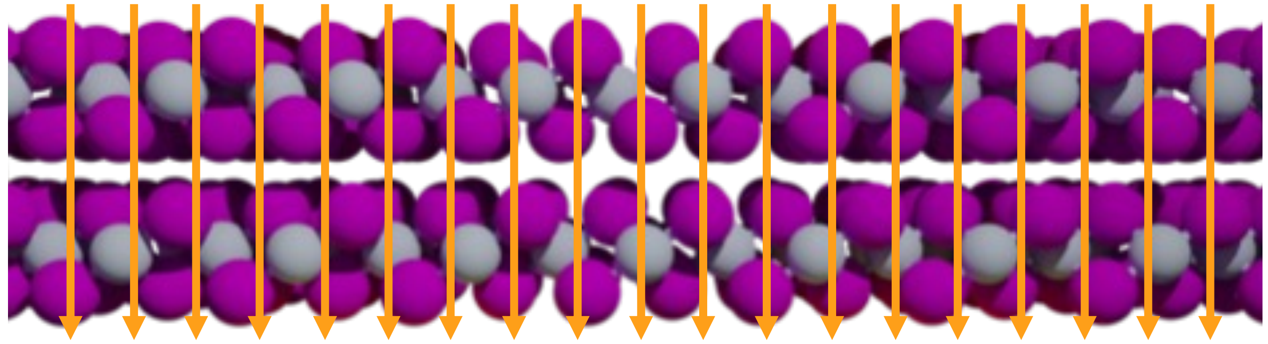
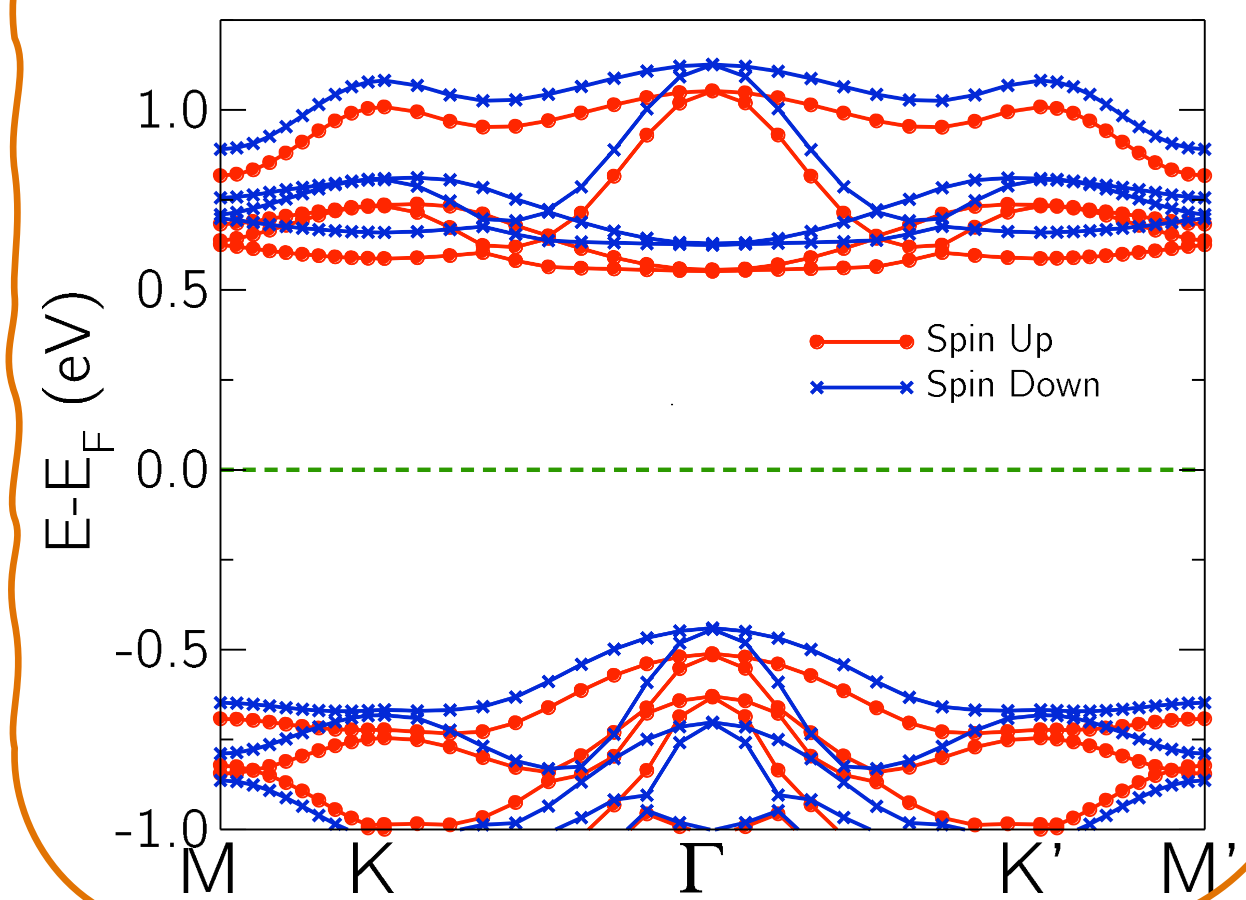


E = 0.4 V/nm



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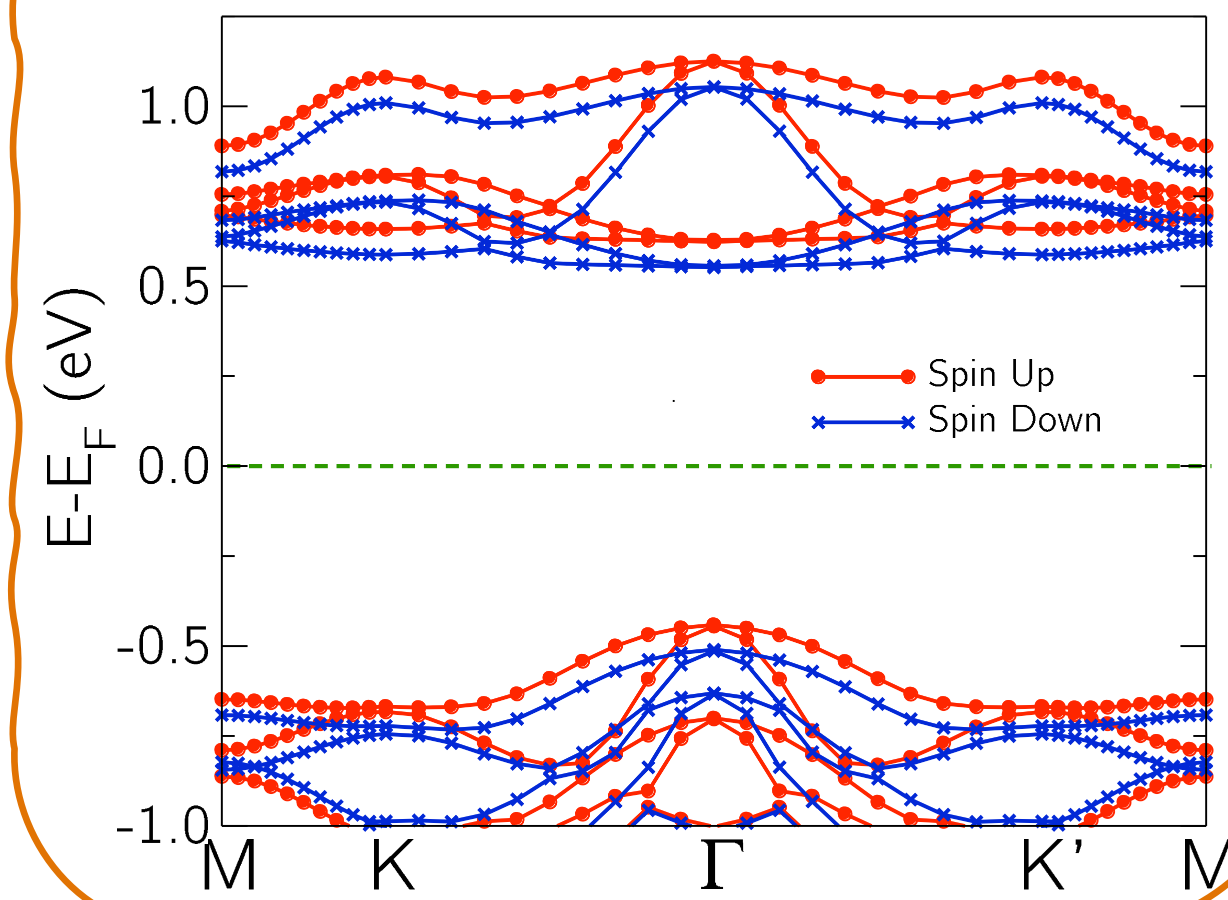

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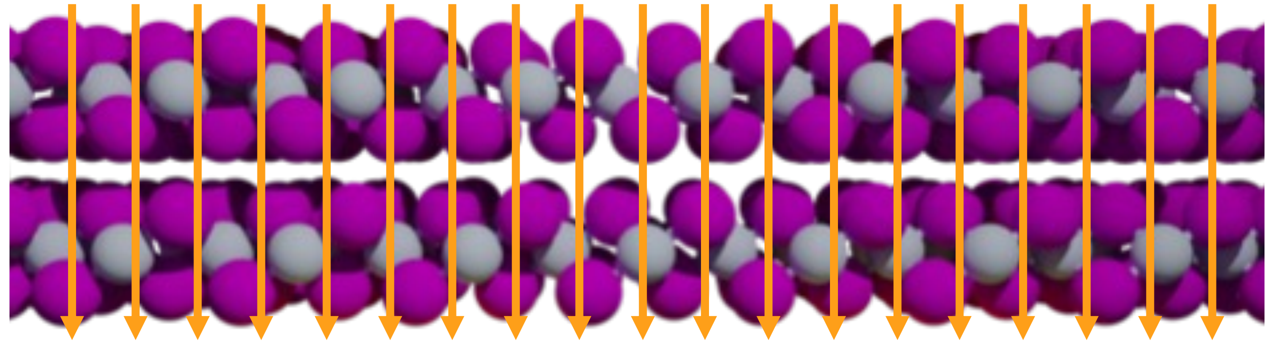

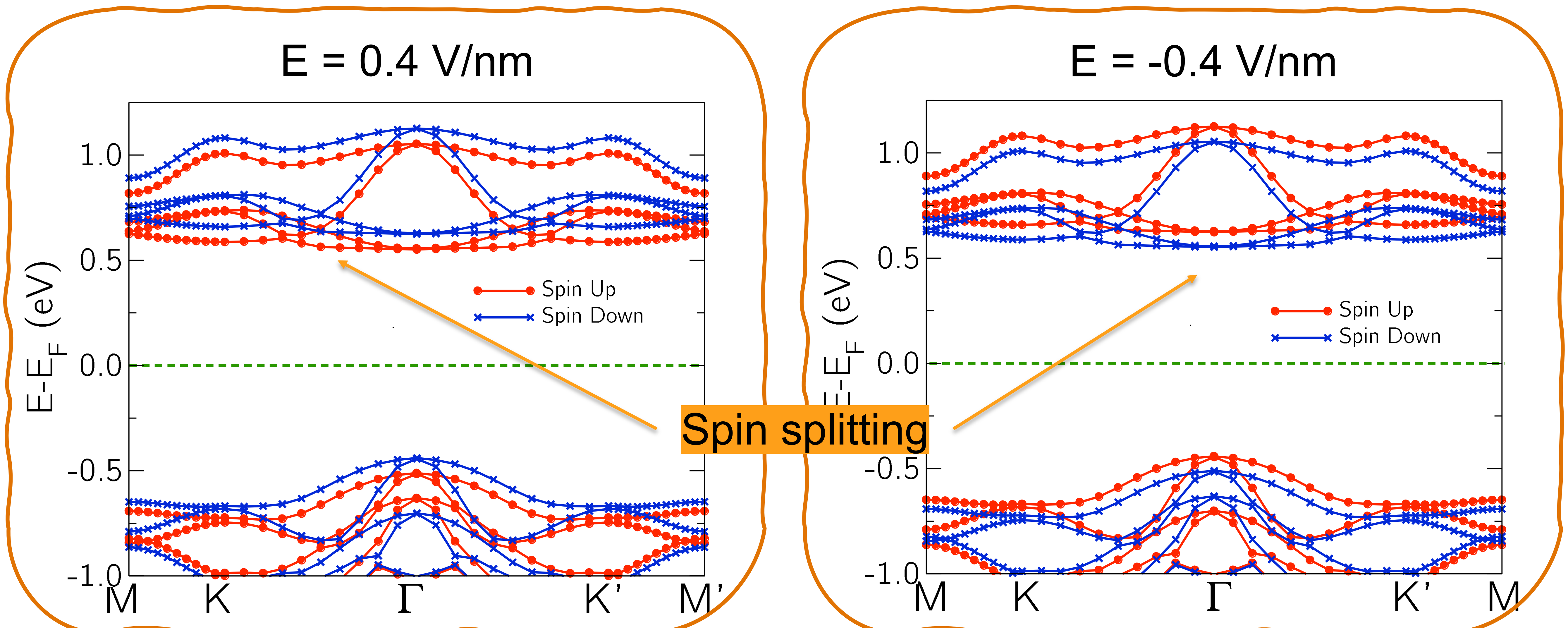

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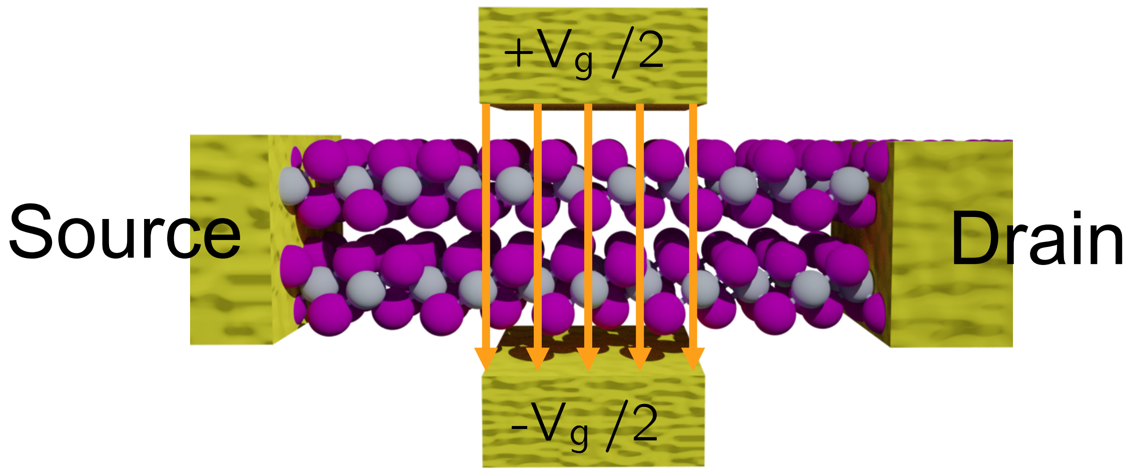
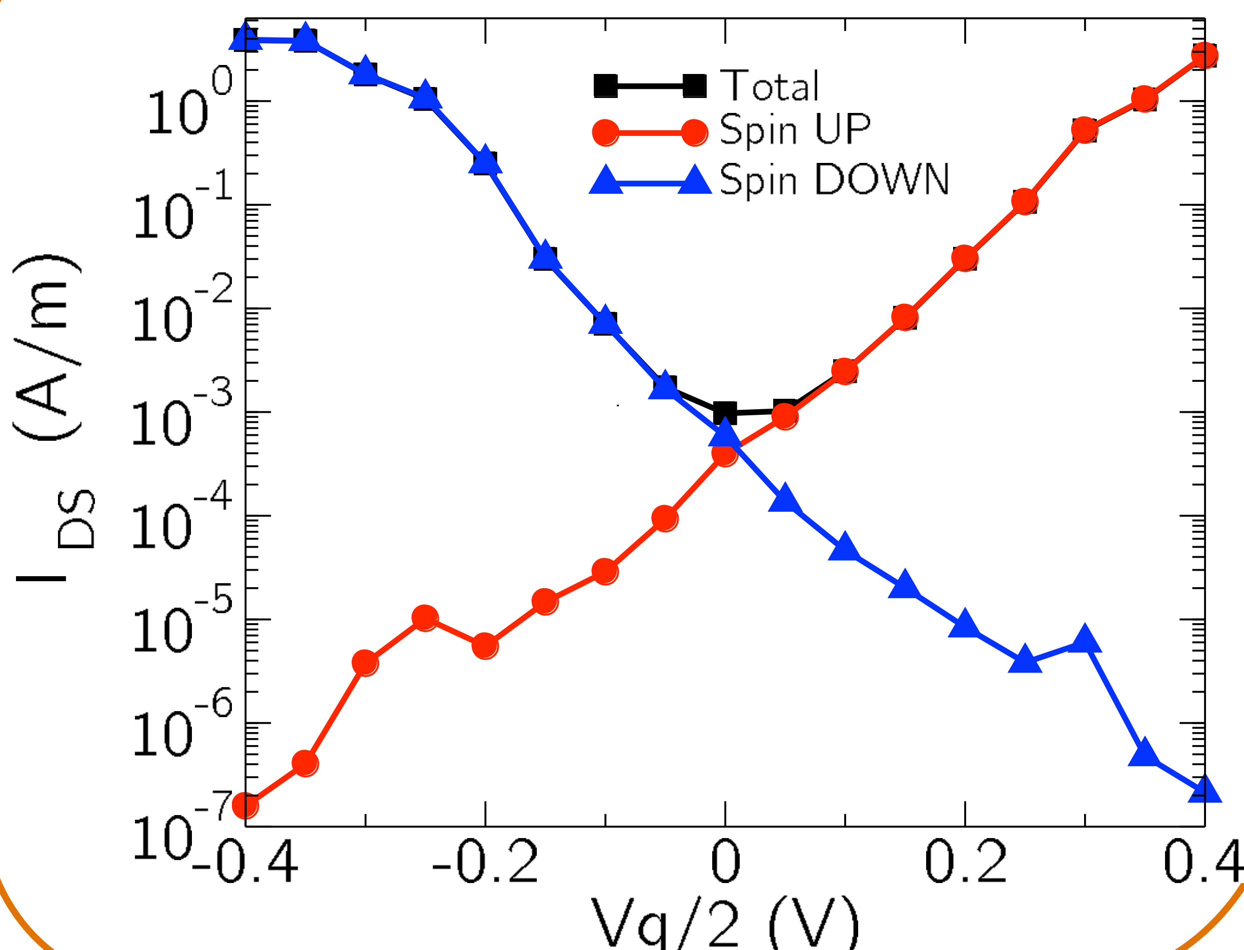
Spin Filter





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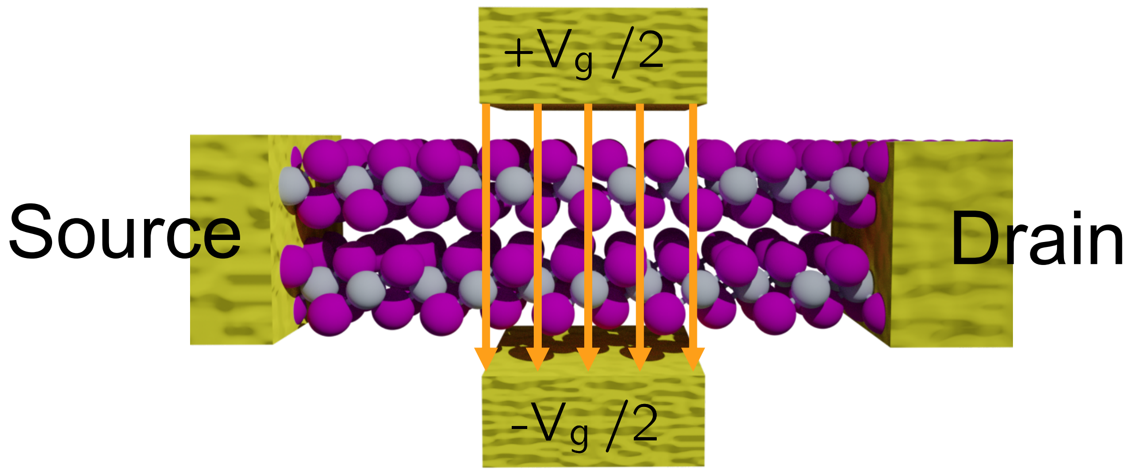
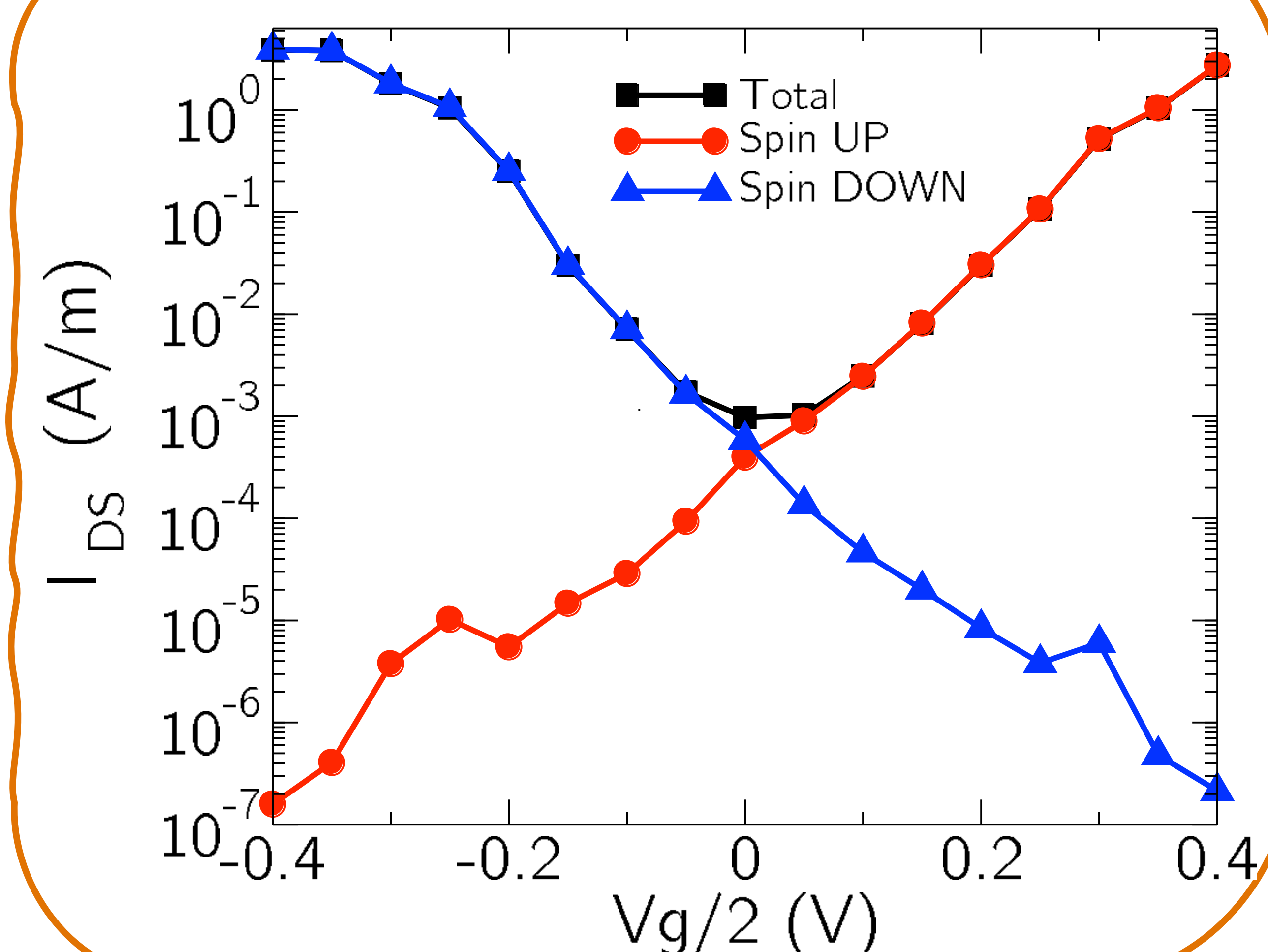
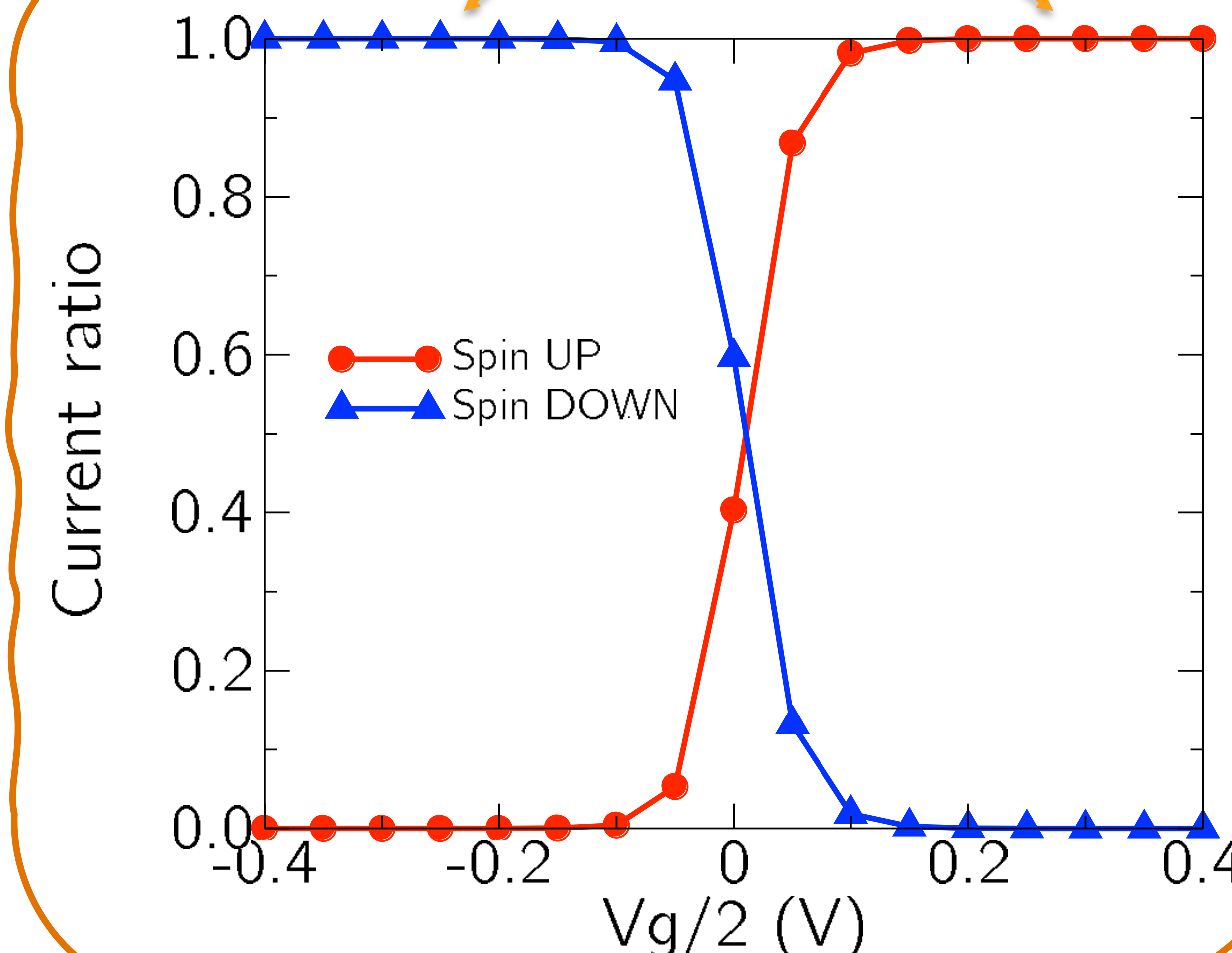


Spin current filtering higher than 99%





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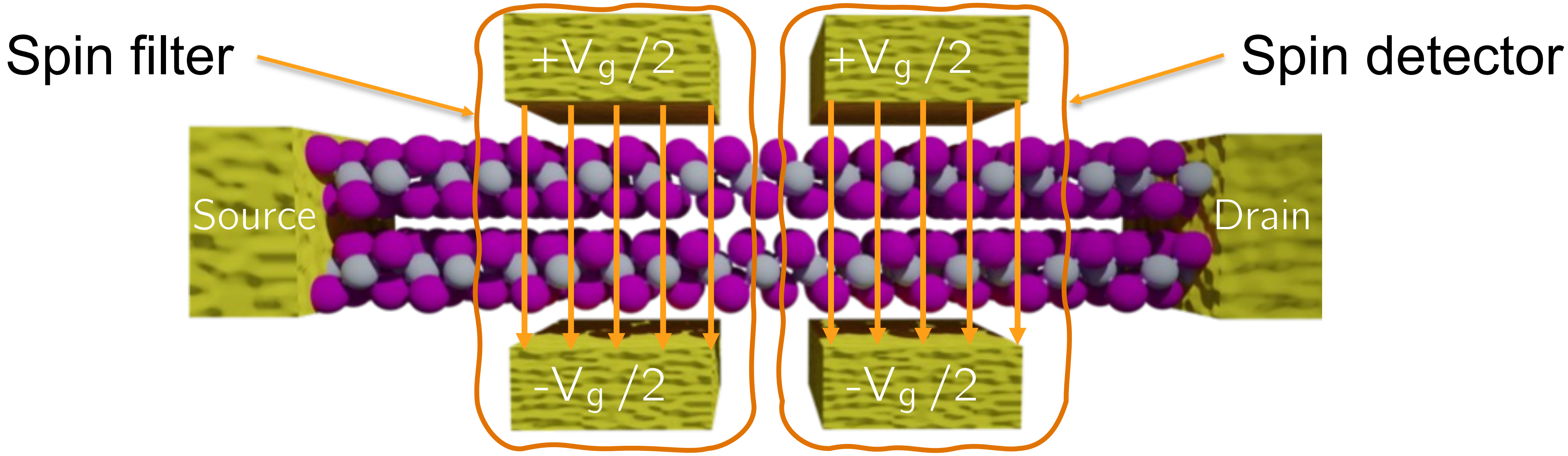
Spin-valve transistor



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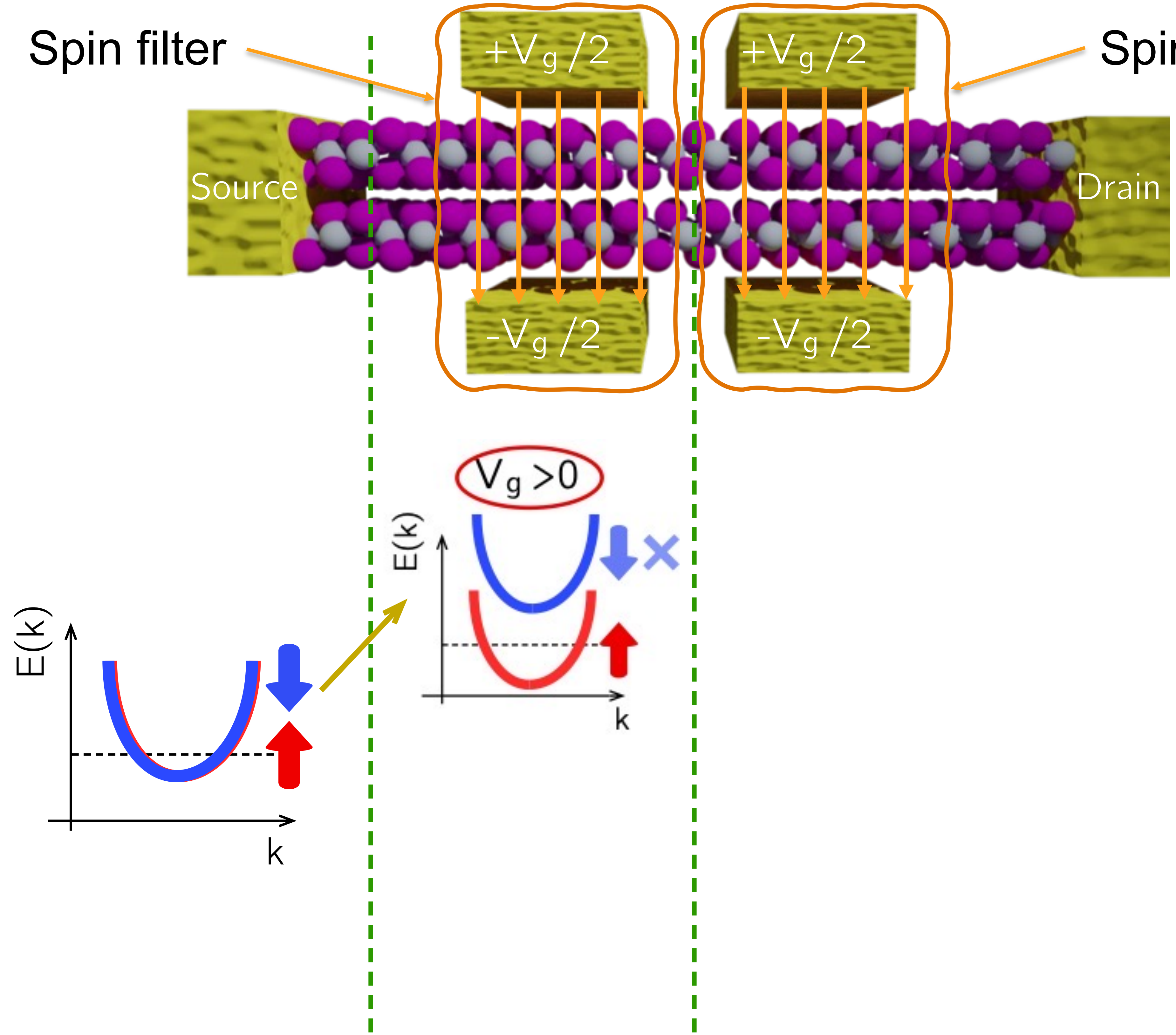

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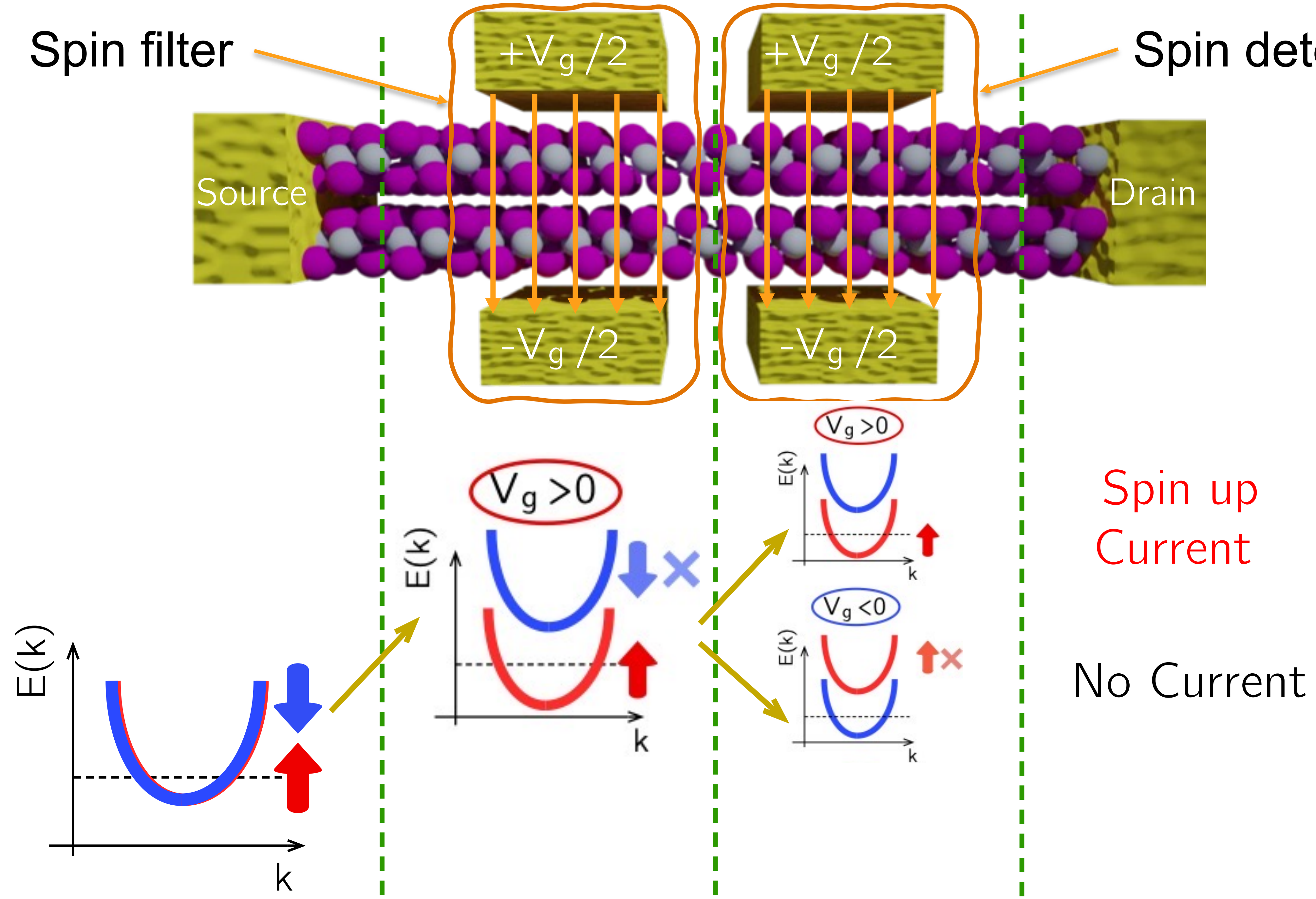

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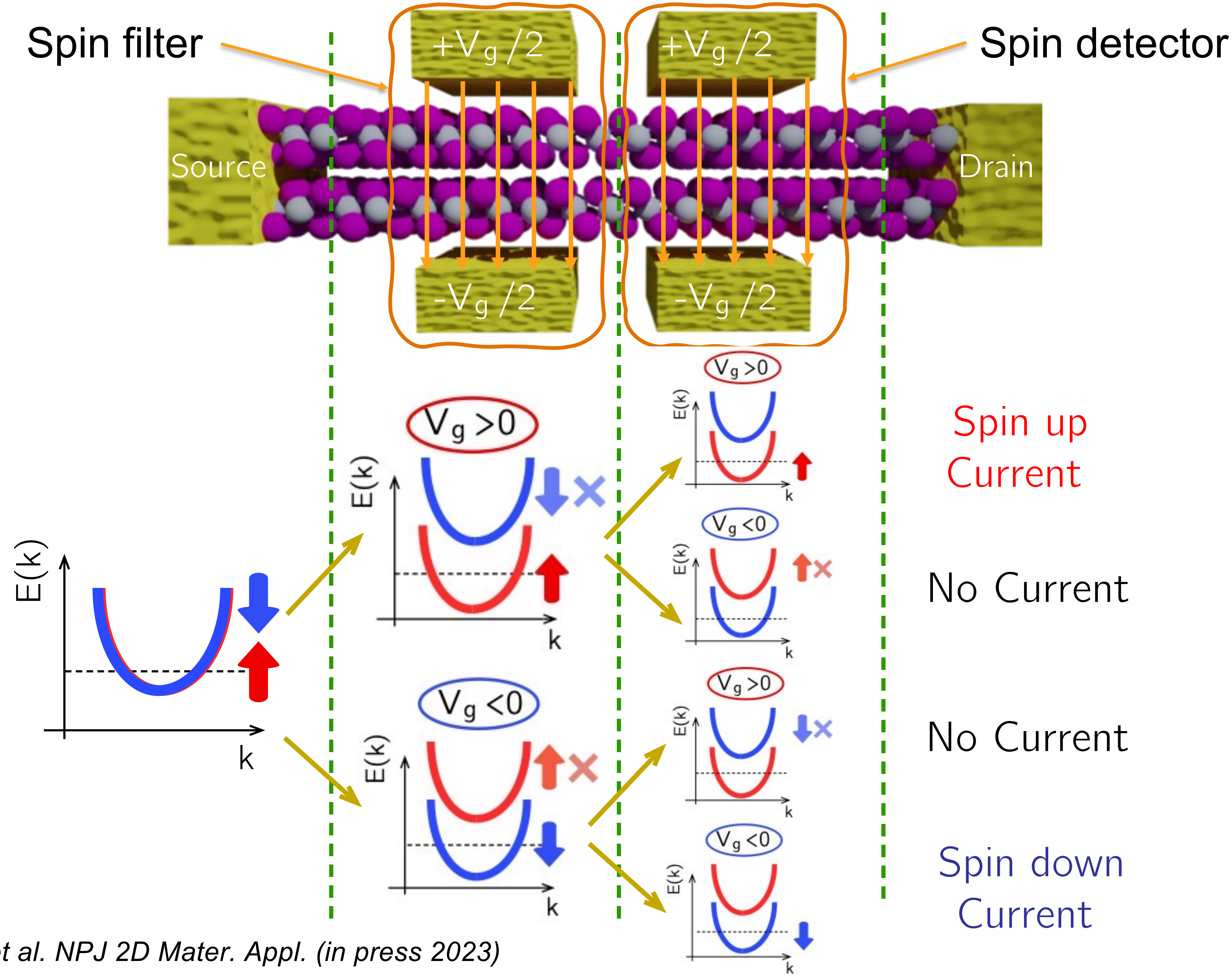

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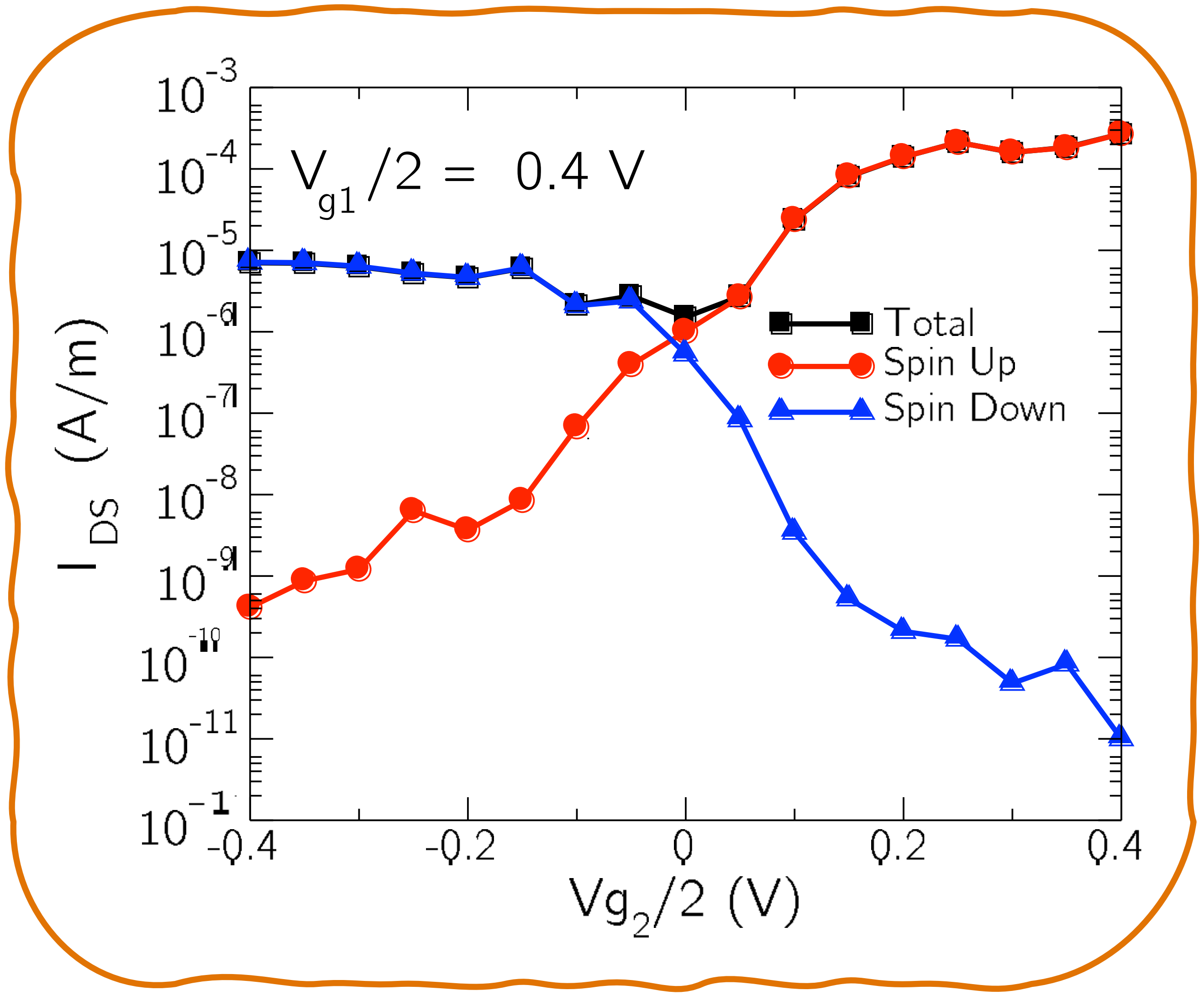

Spin polarization up to 99%

ON/OFF current ratio (~ 10^2)

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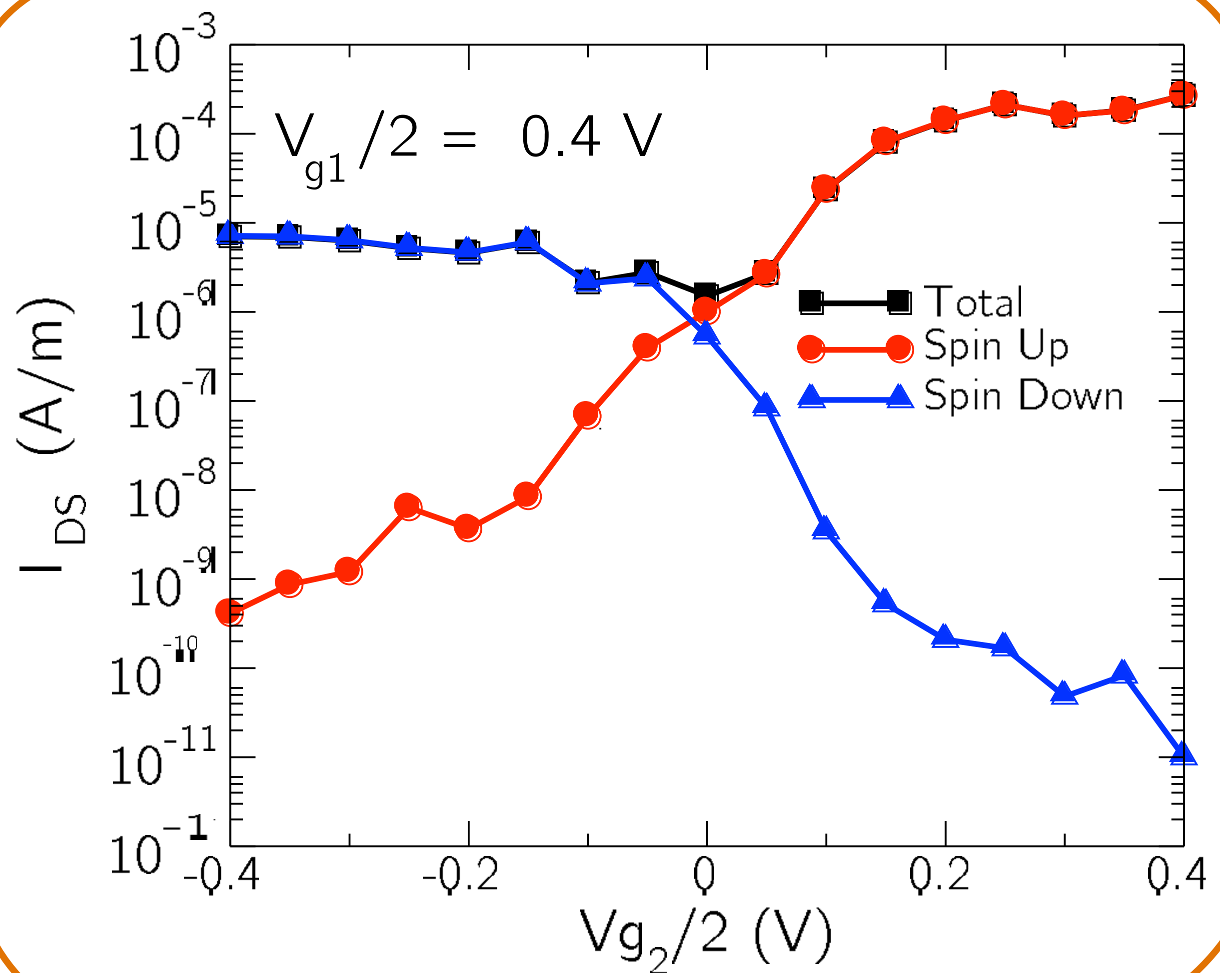
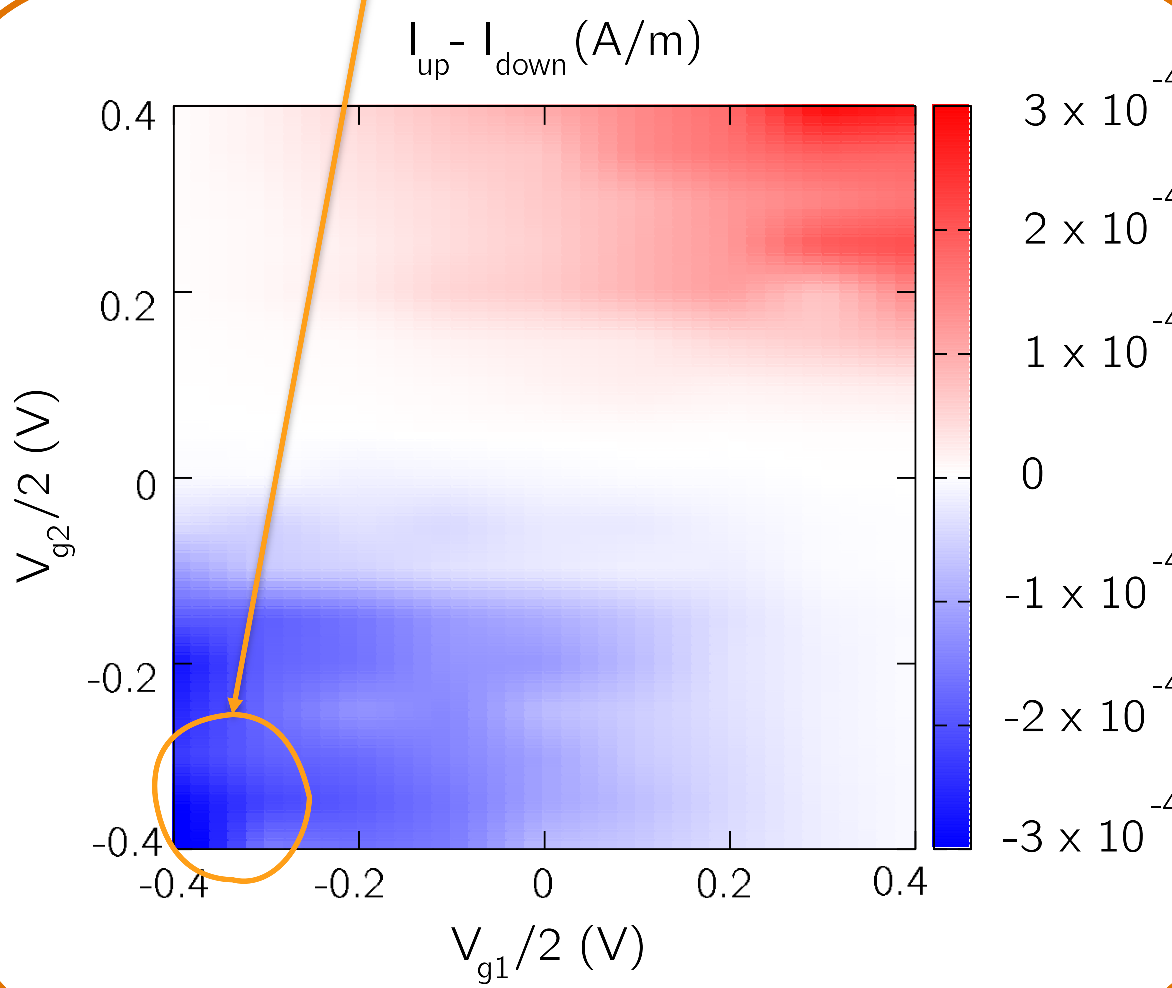
Spin-valve transistor



Tuning the two gate regions, it is possible to select between *down*, *up*, and *zero* spin polarized current



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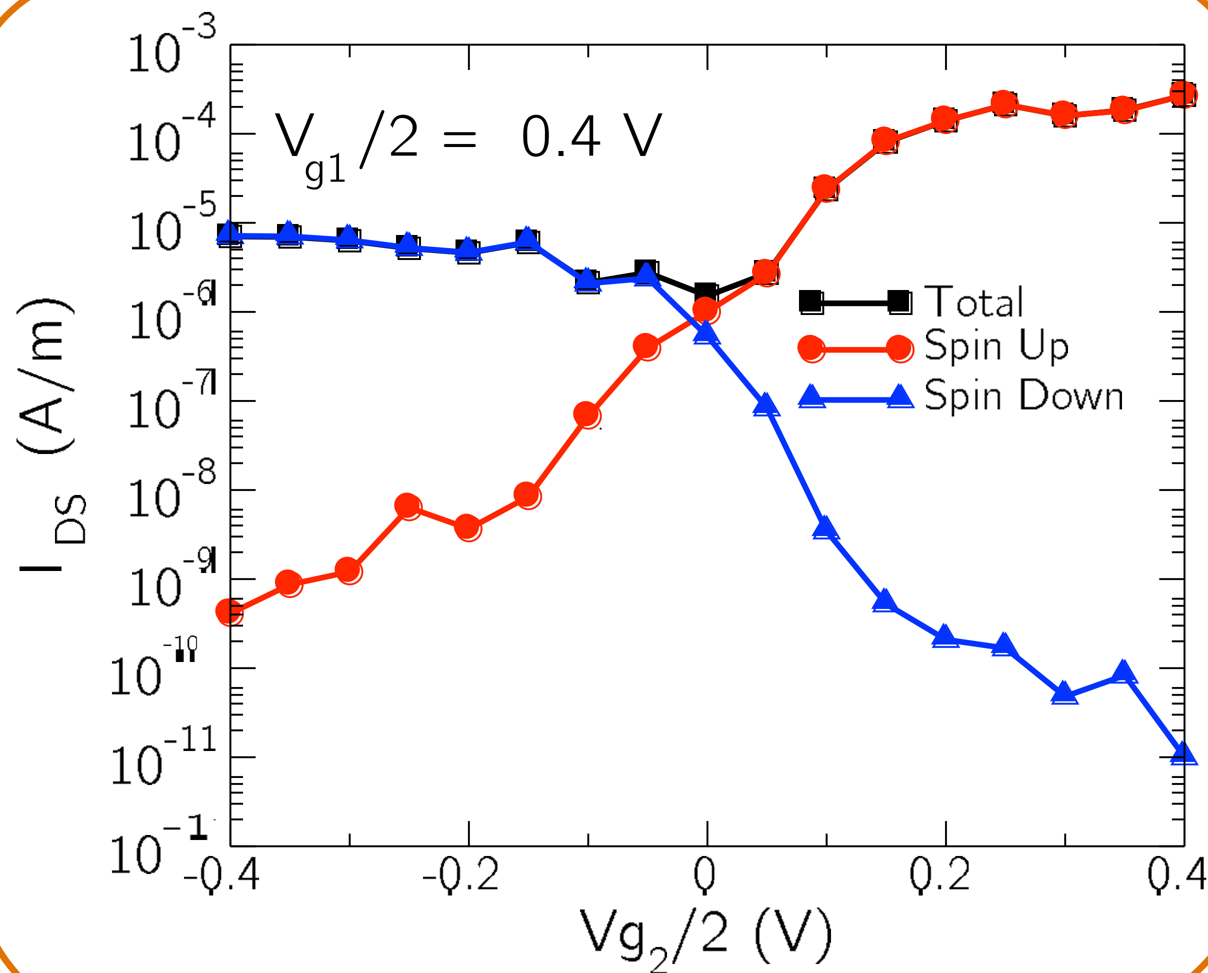

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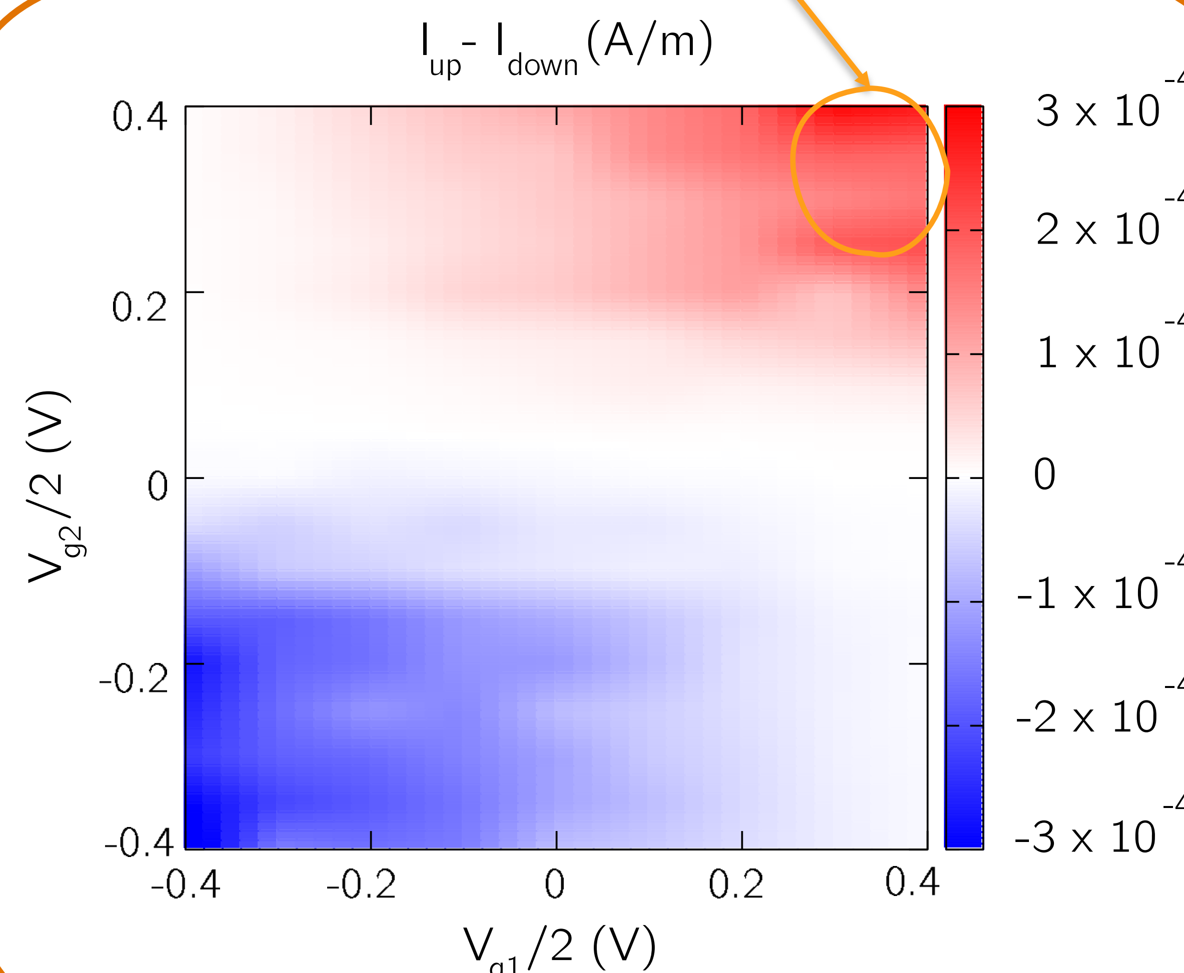

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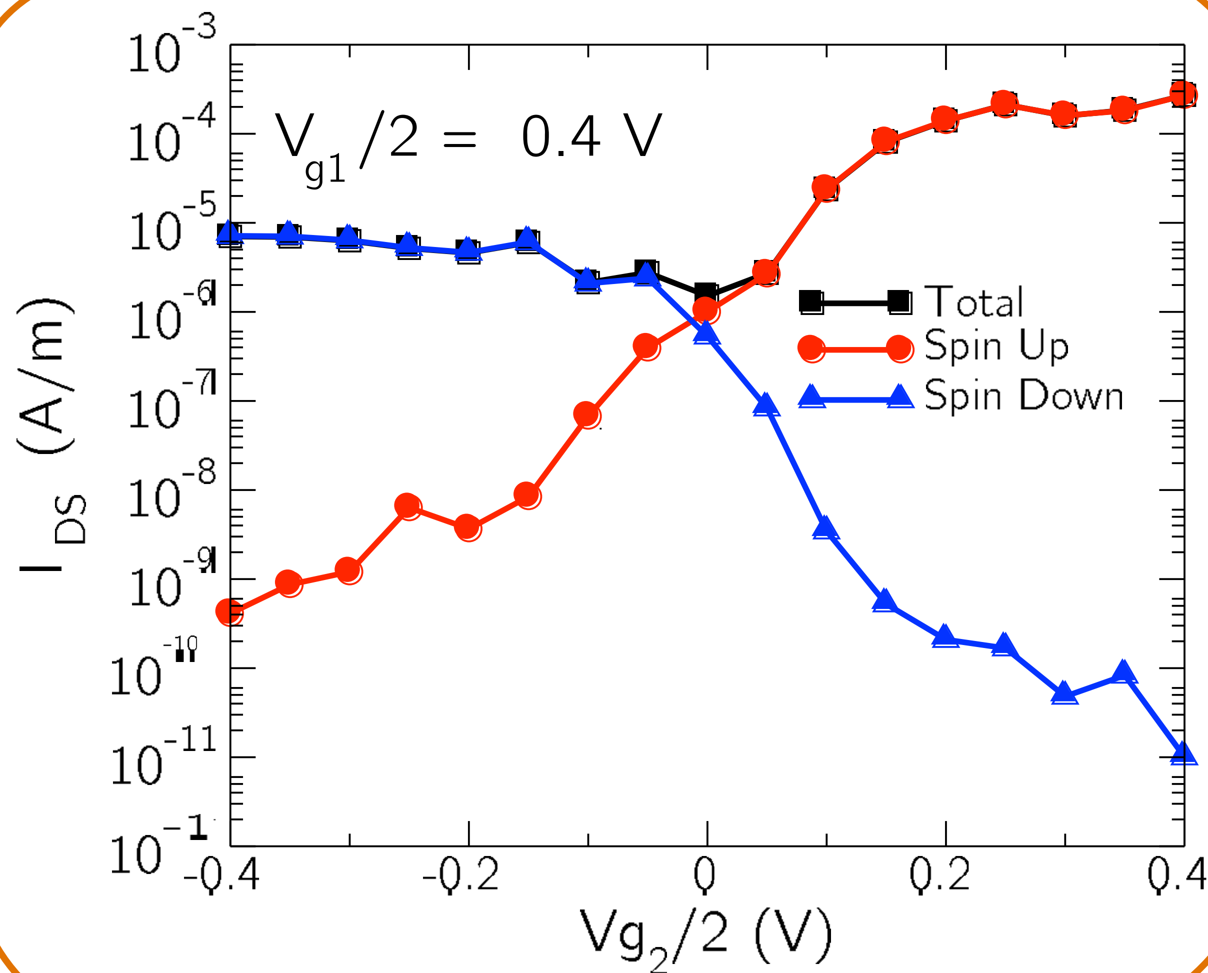

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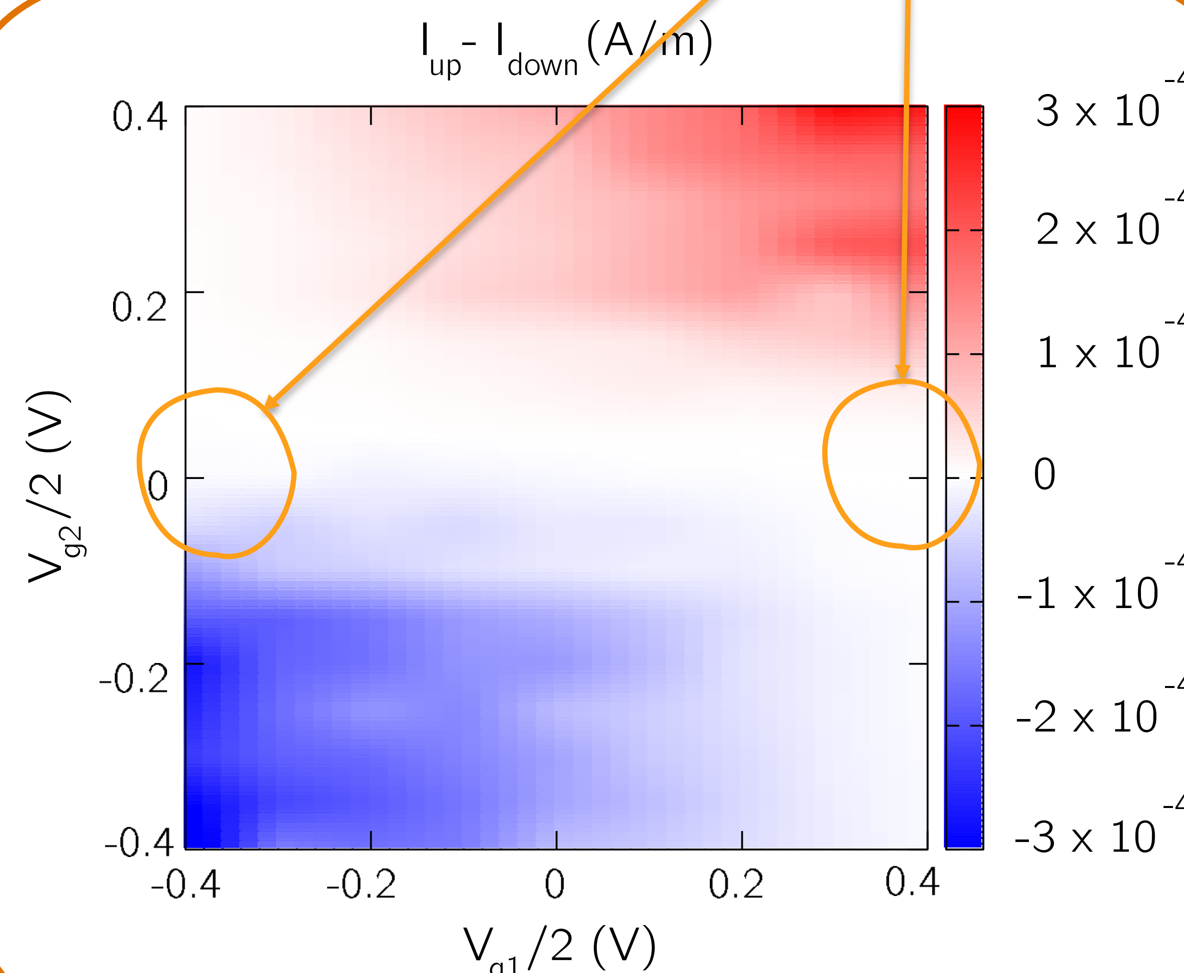

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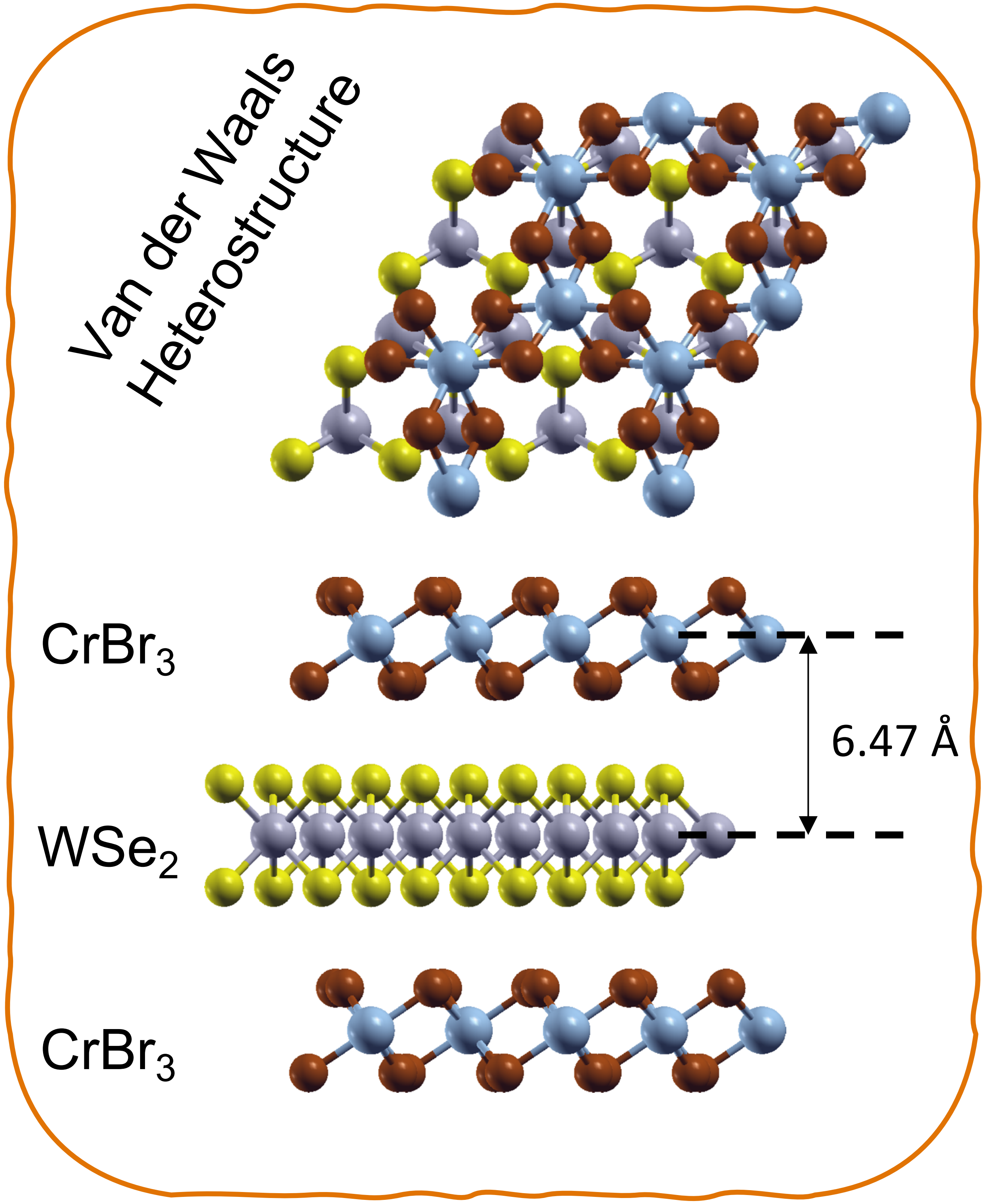
$CrBr_3/WSe_2/CrBr_3$ vdW HS



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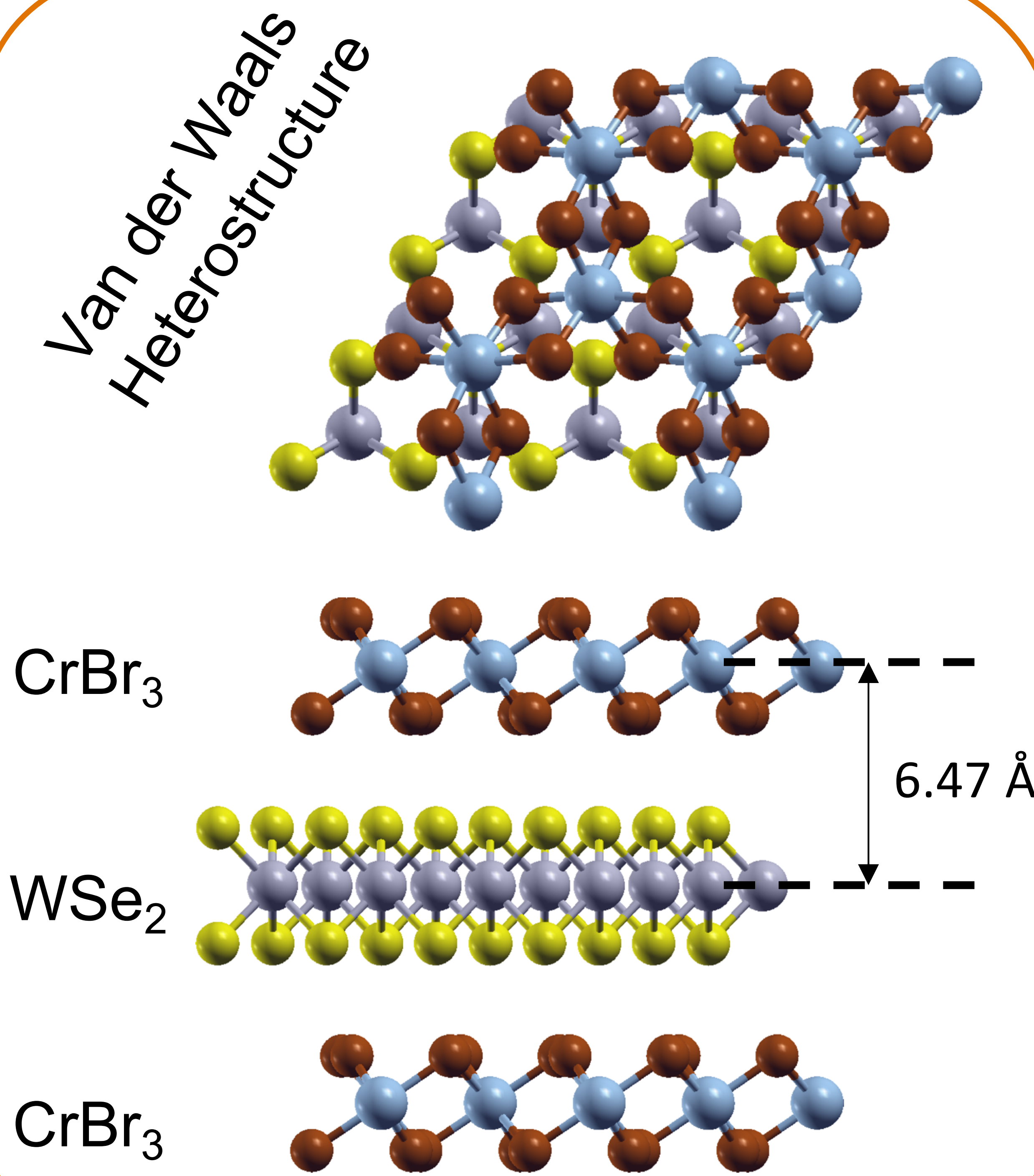
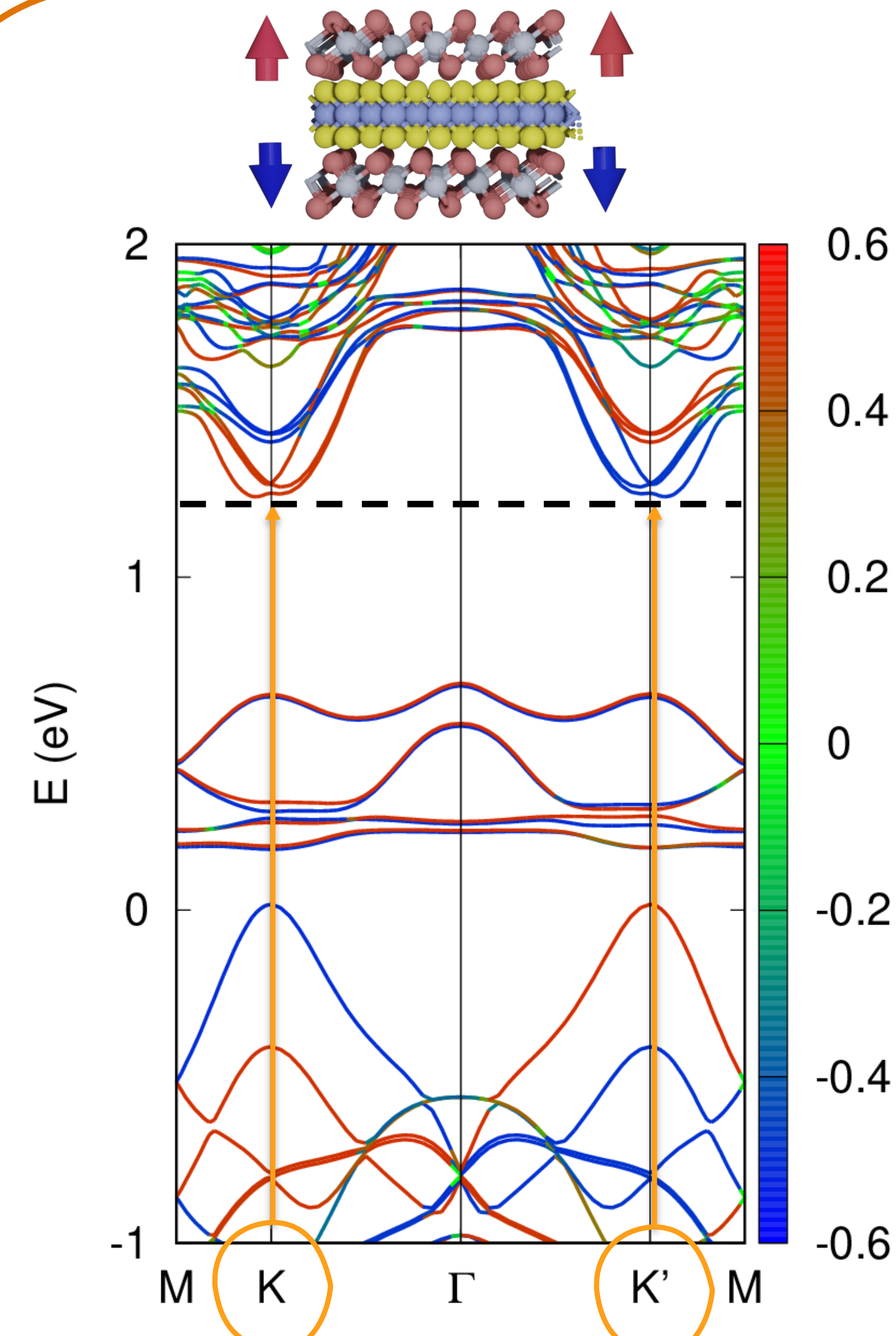
$CrBr_3/WSe_2/CrBr_3$ vdW HS





No valley splitting

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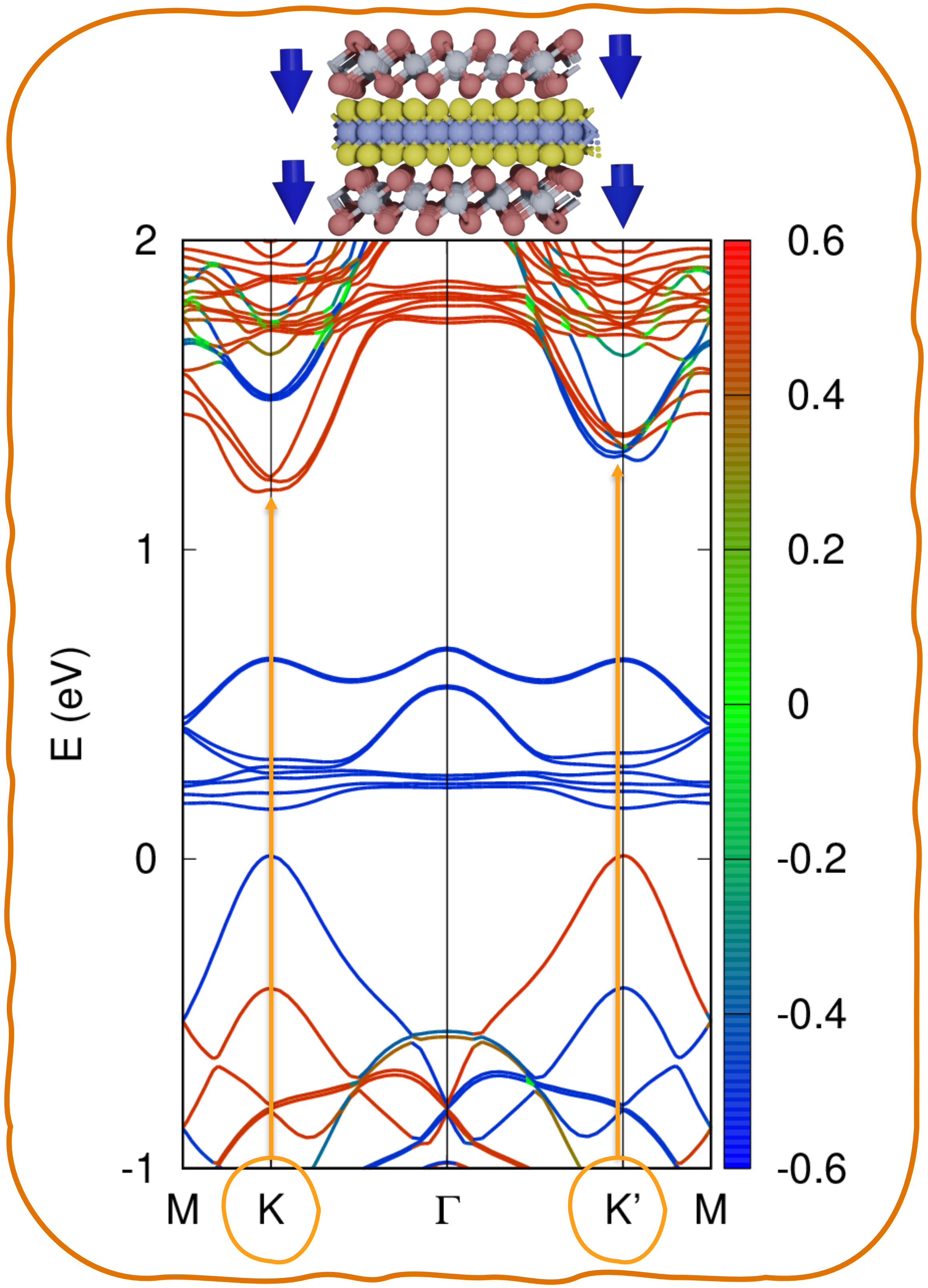
$CrBr_3/WSe_2/CrBr_3$ vdW HS



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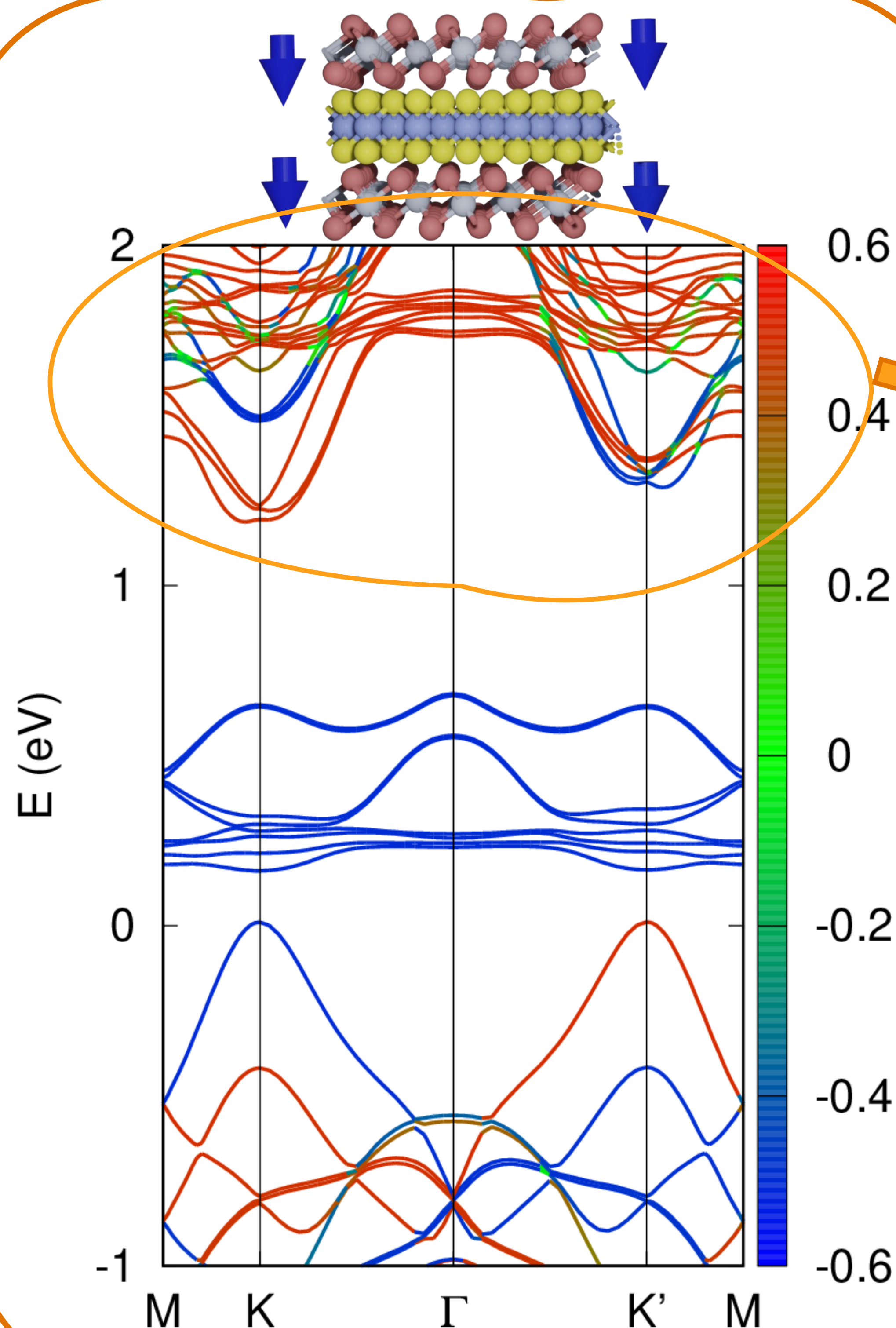

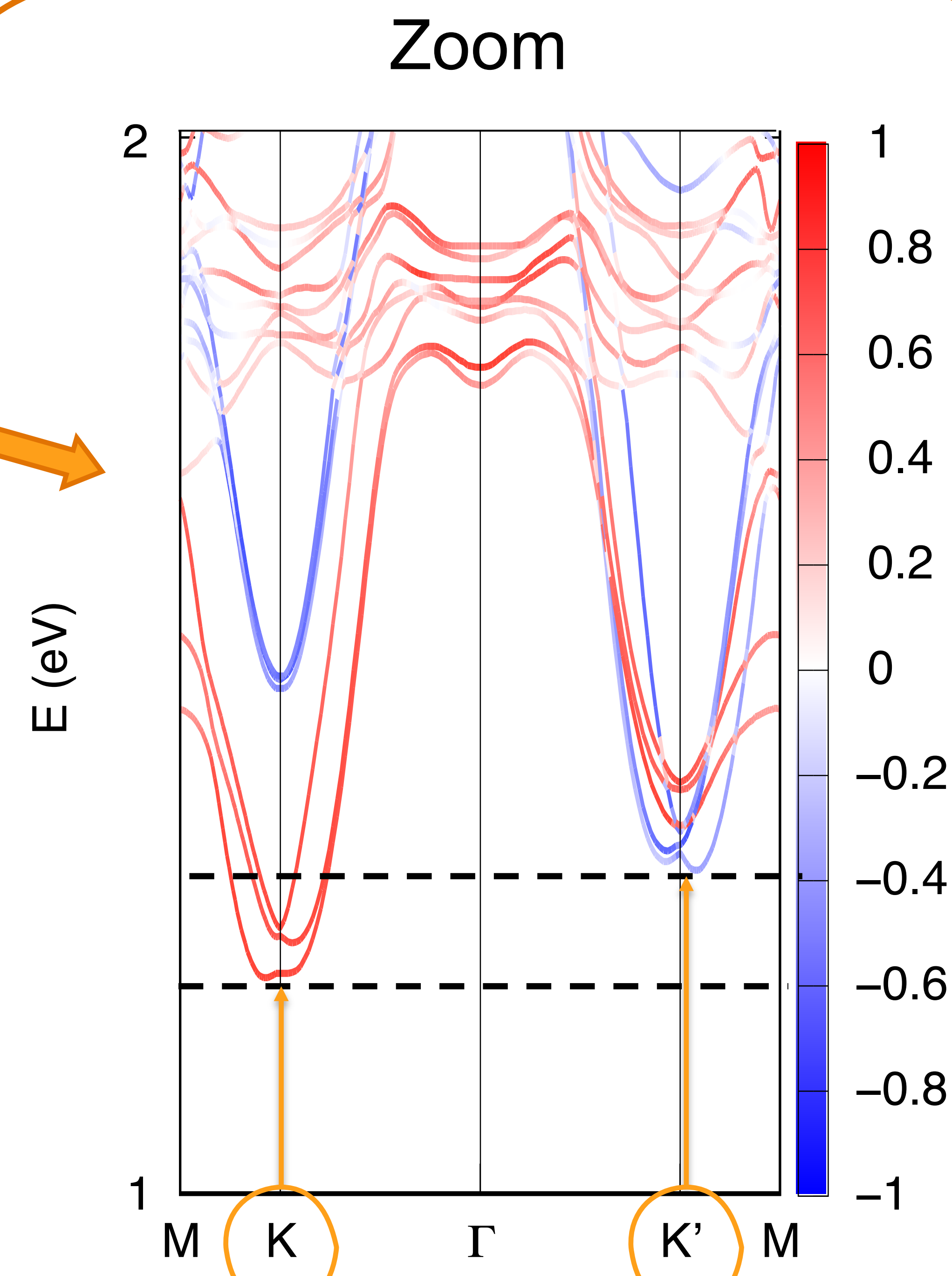

Valley splitting of ~ 100 meV

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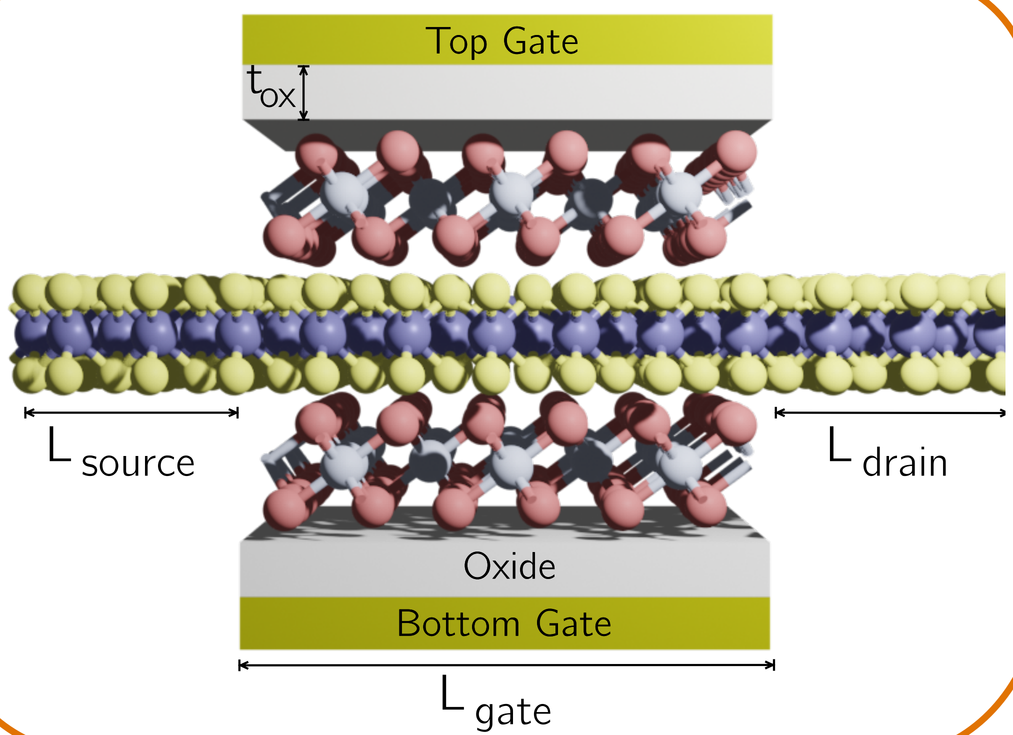
Valleytronic device



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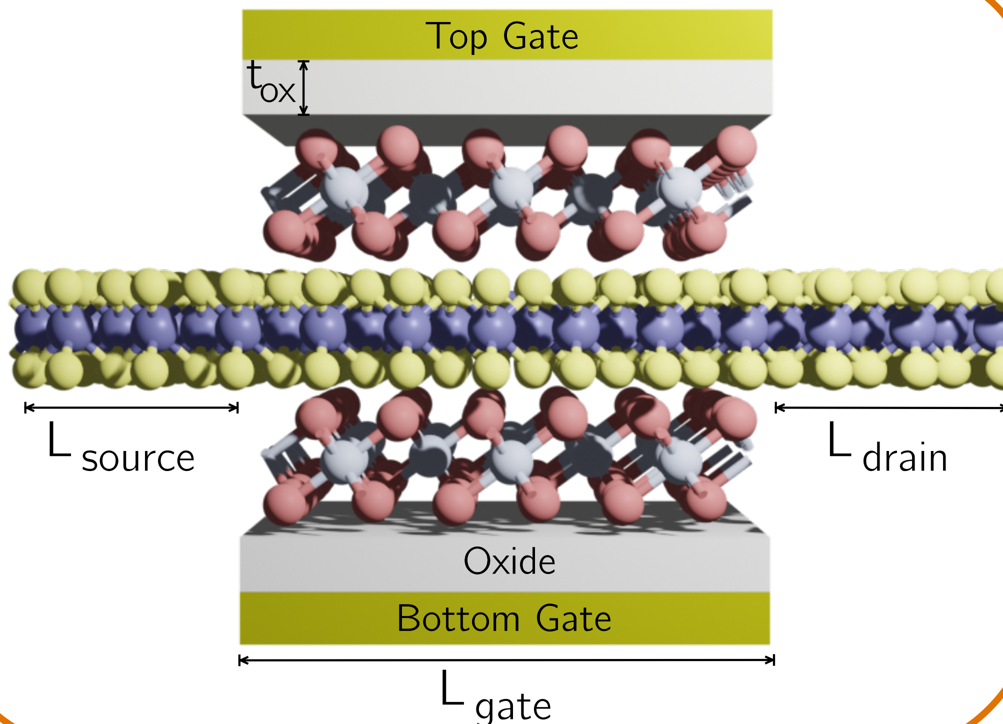

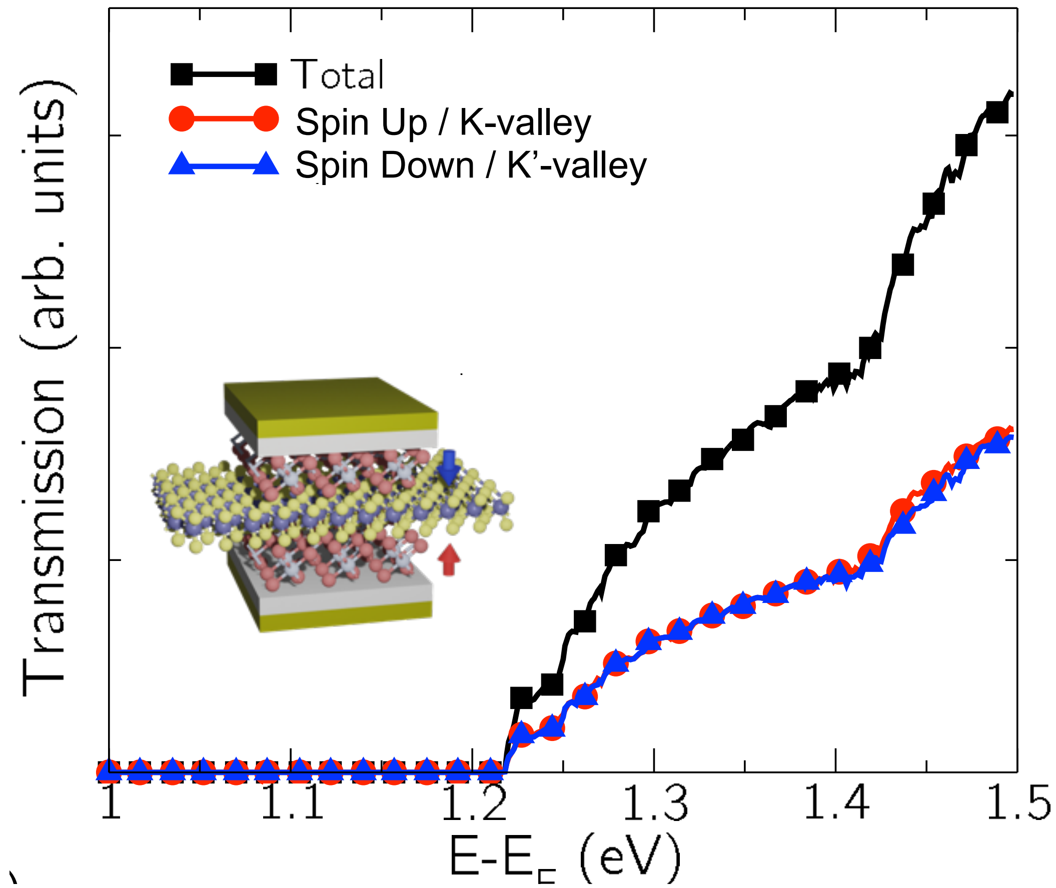

Counter-polarized

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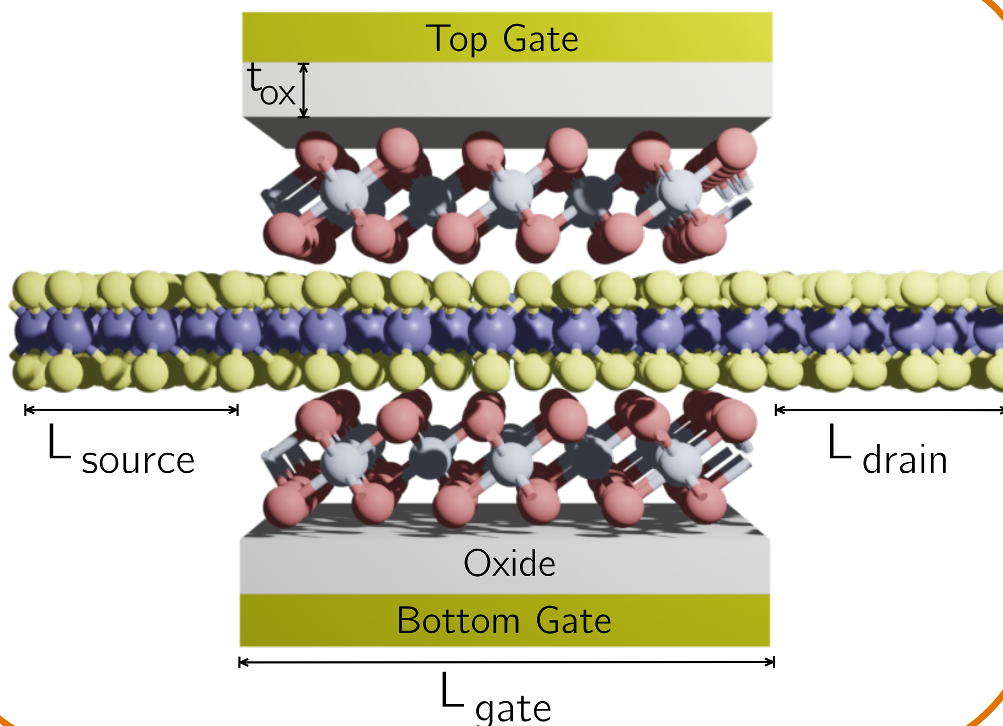
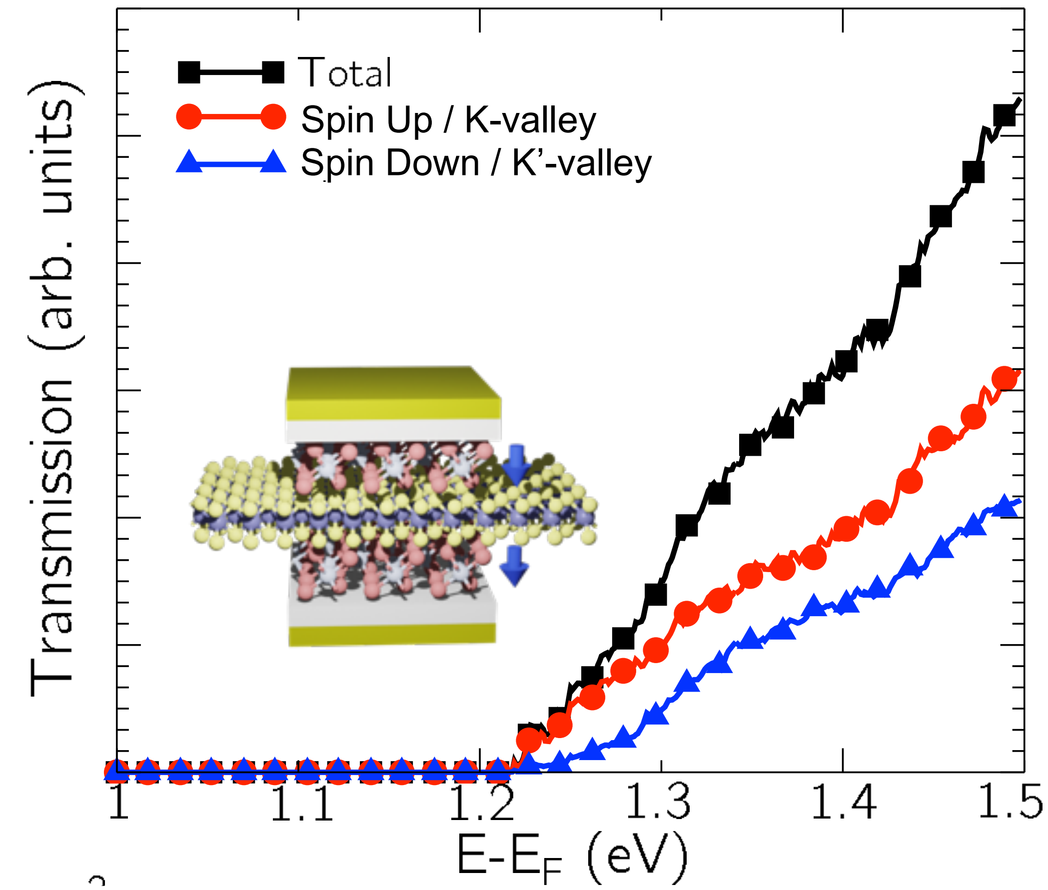
Valleytronic device





Co-polarized

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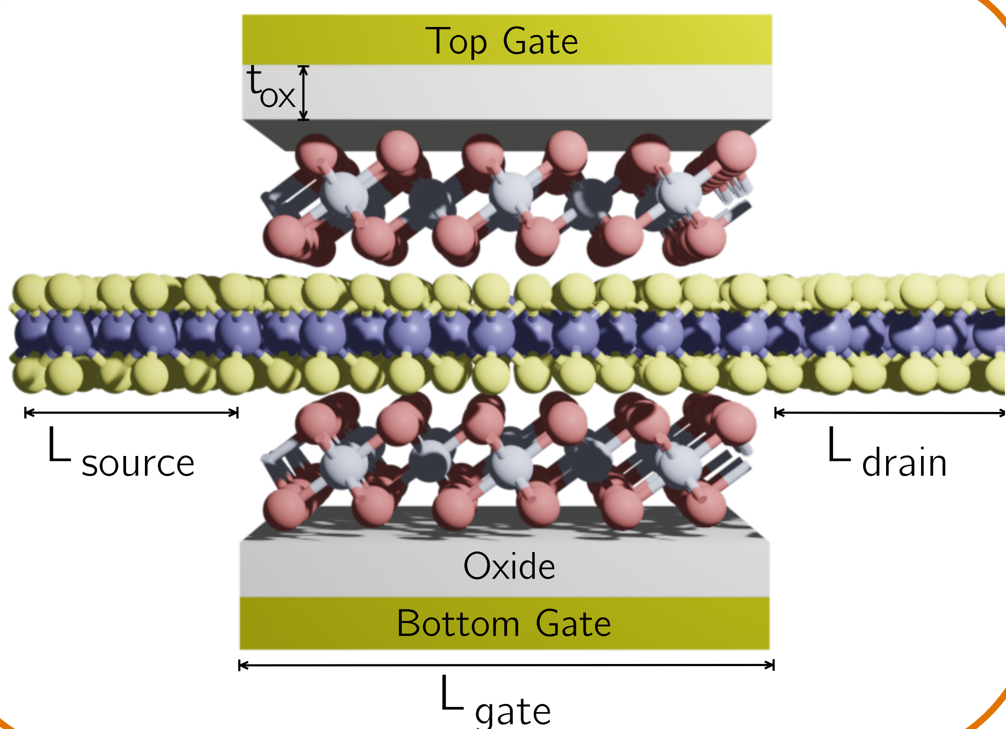
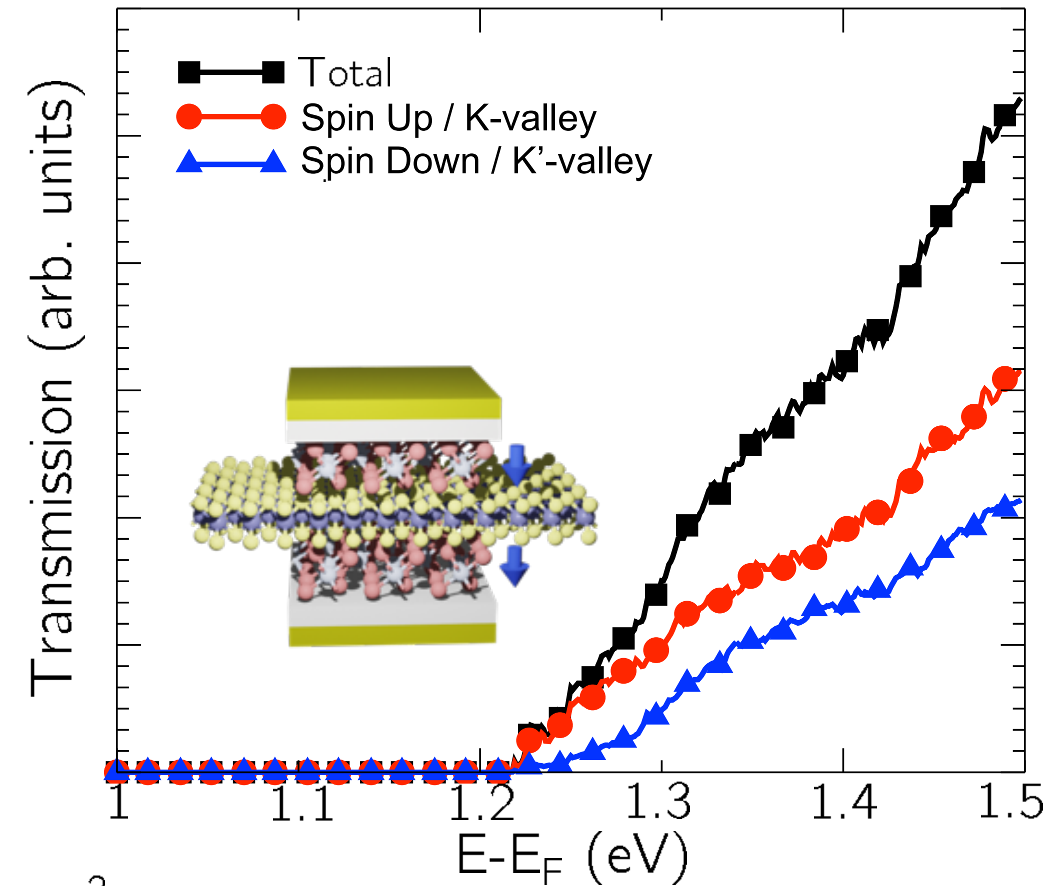
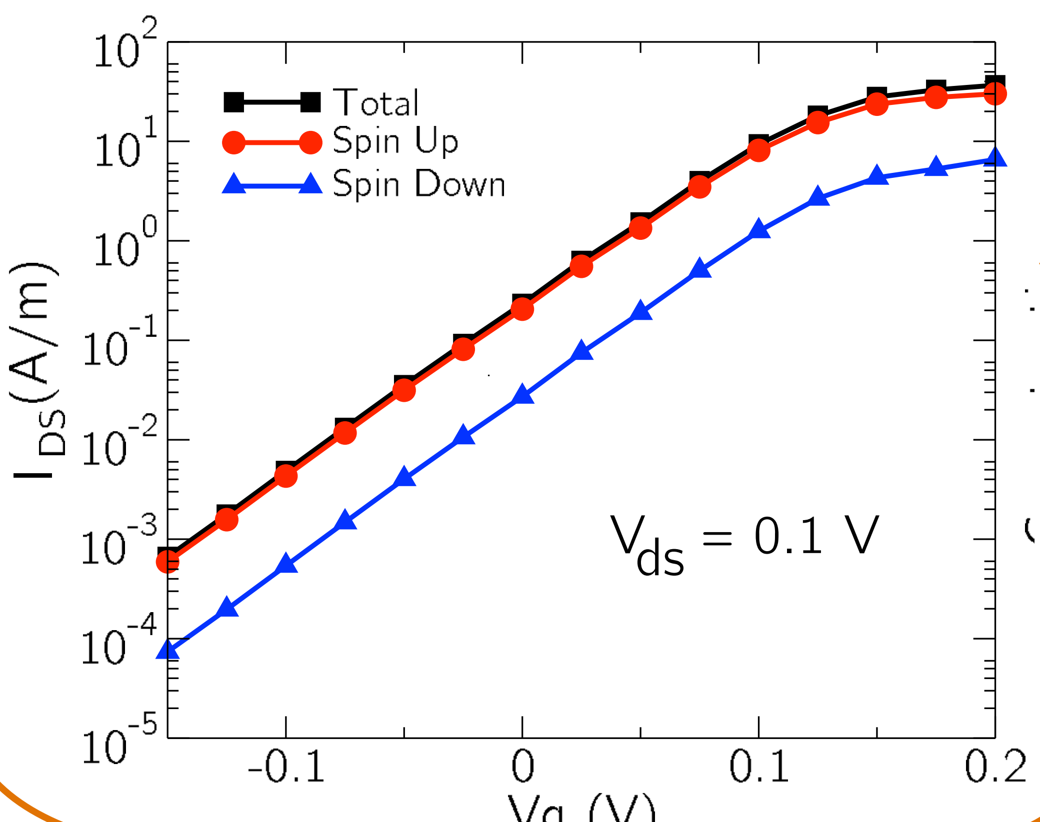
Valleytronic device







Transfer characteristic

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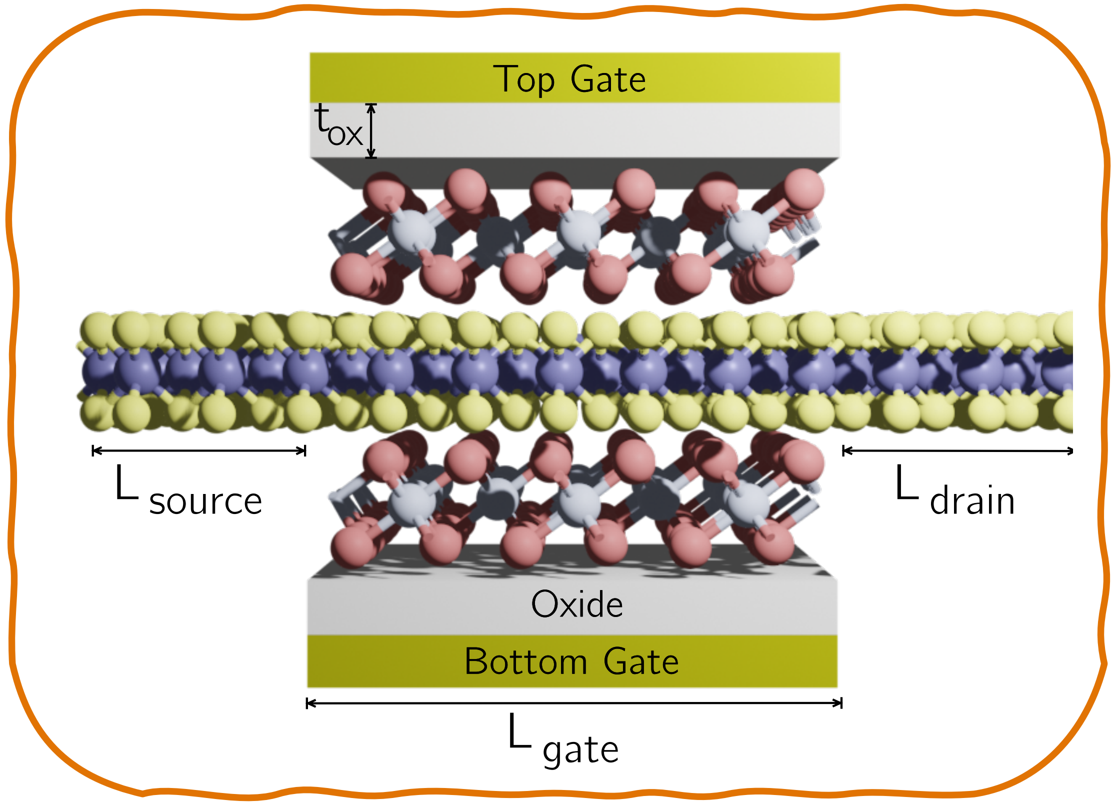
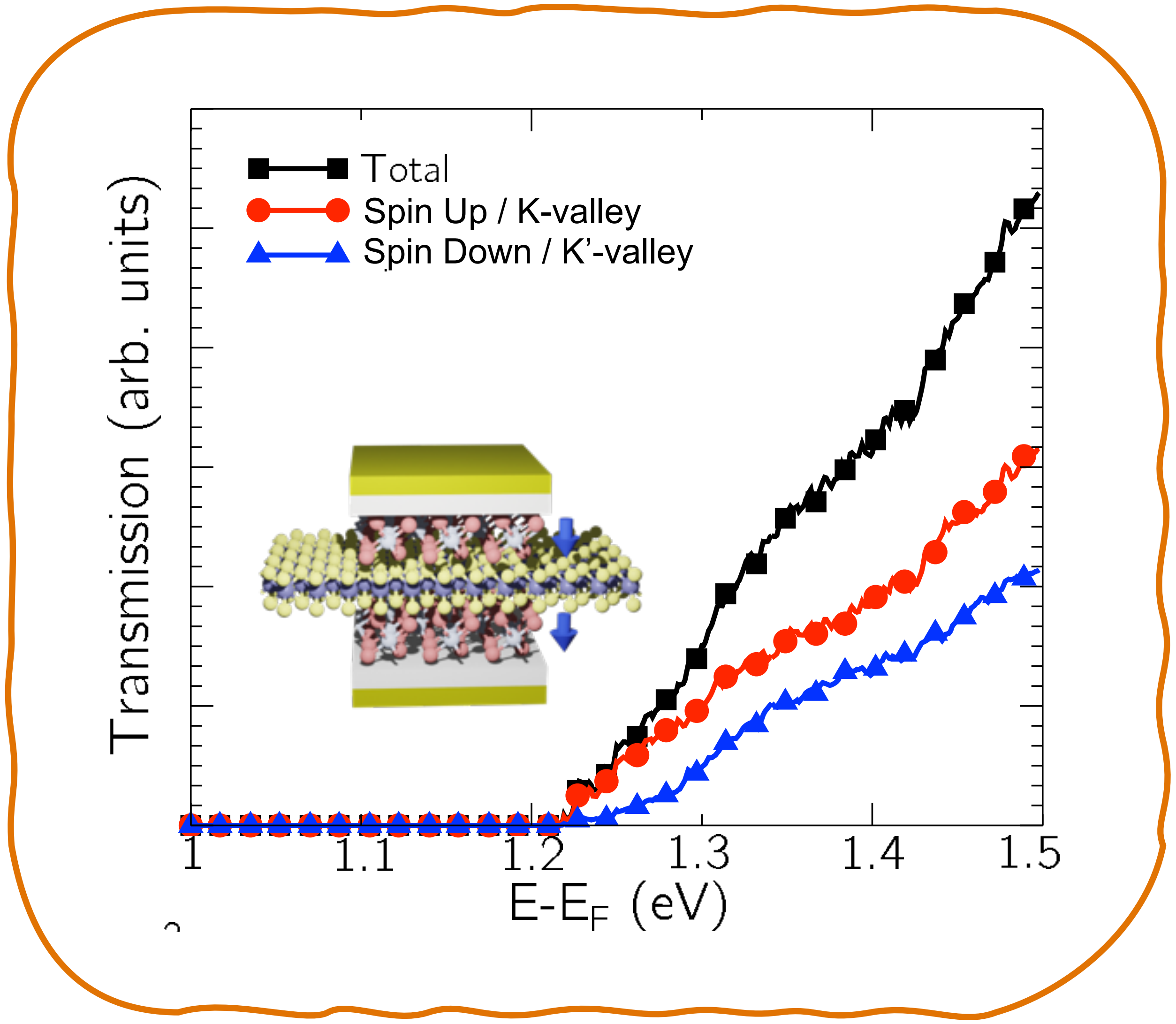
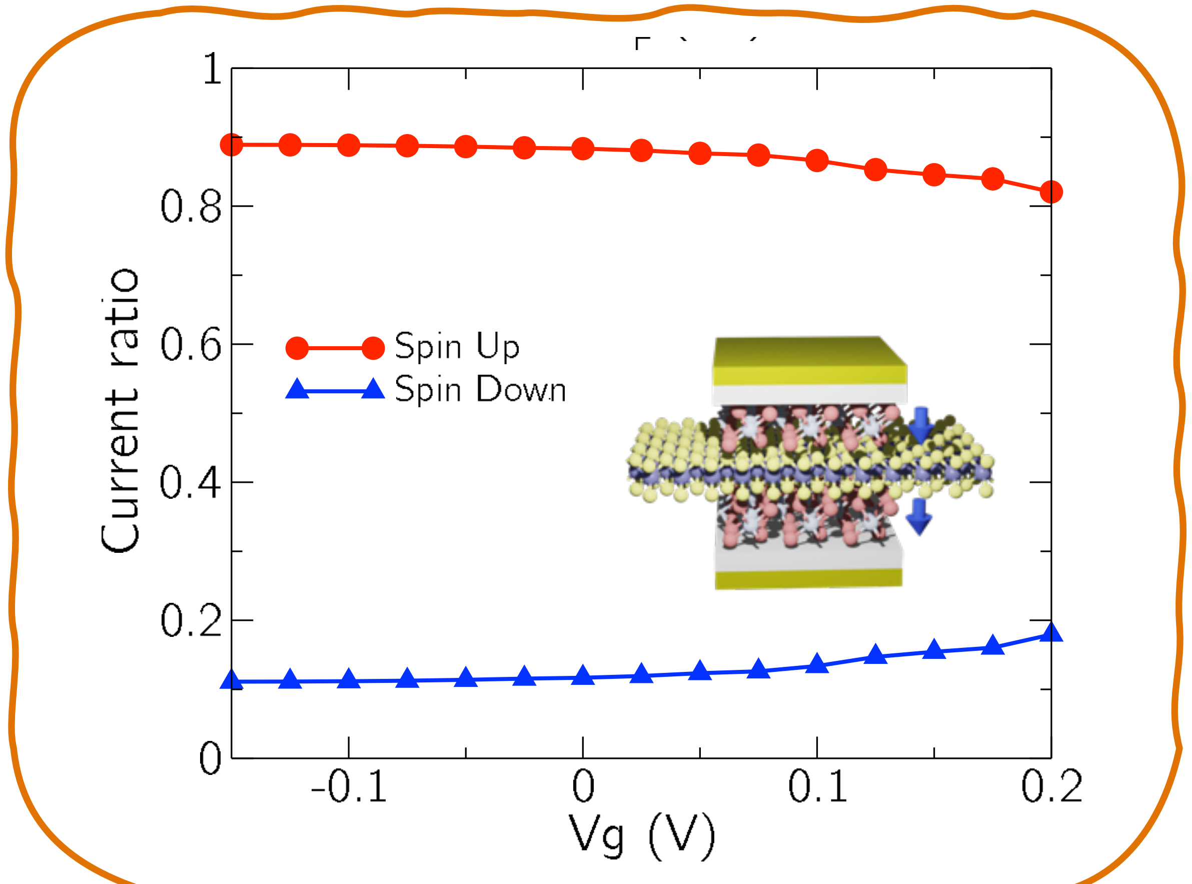
Valleytronic device







Spin/valley polarization is always larger than 80%

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Acknowledgments

GRAPHENE
FLAGSHIP

Graphene Flagship Core 3 (Co. # 881603)

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IWCN - 13th June 2023

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Spin-valley transport in magnetic 2D materials through multiscale simulations

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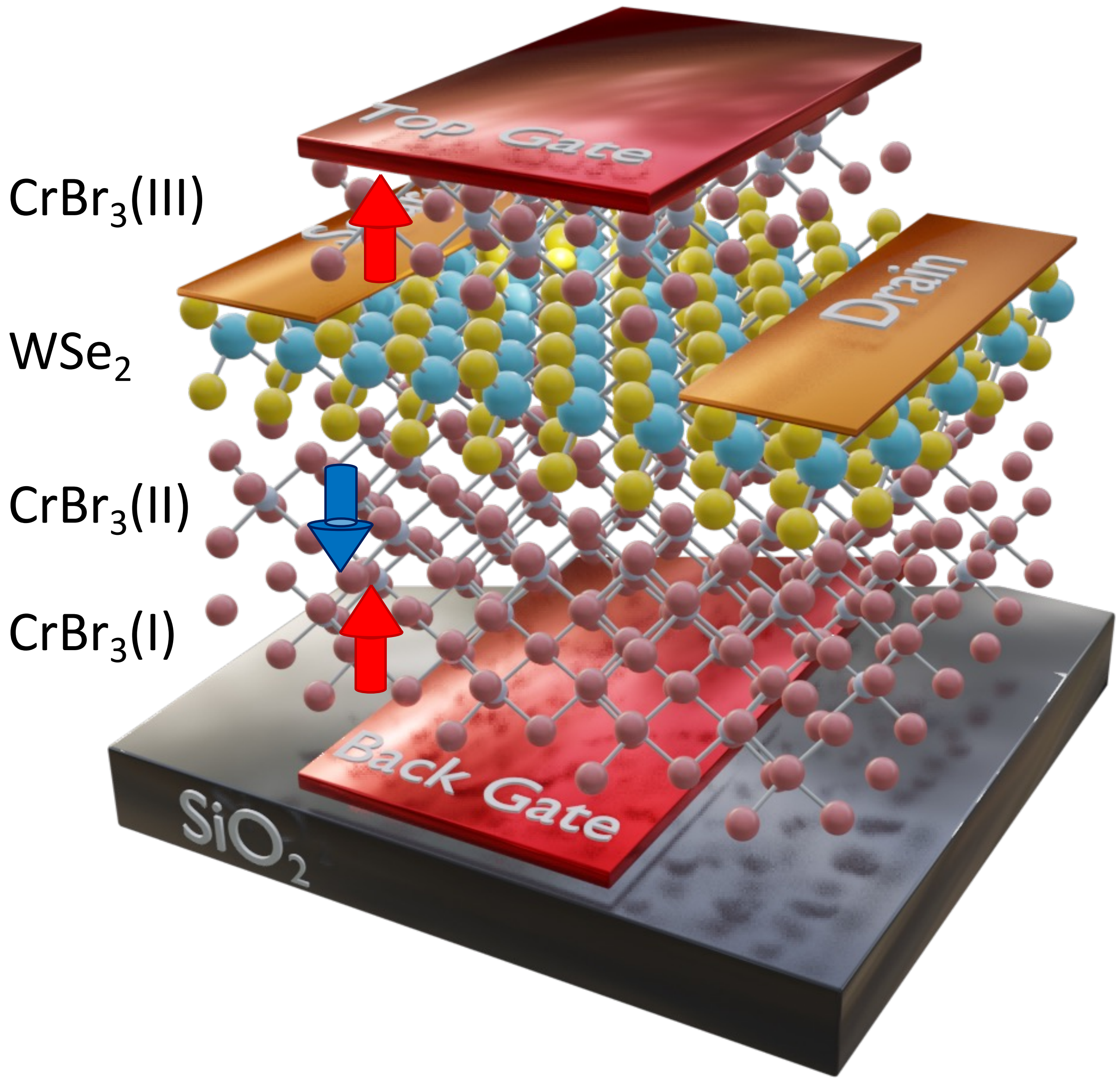
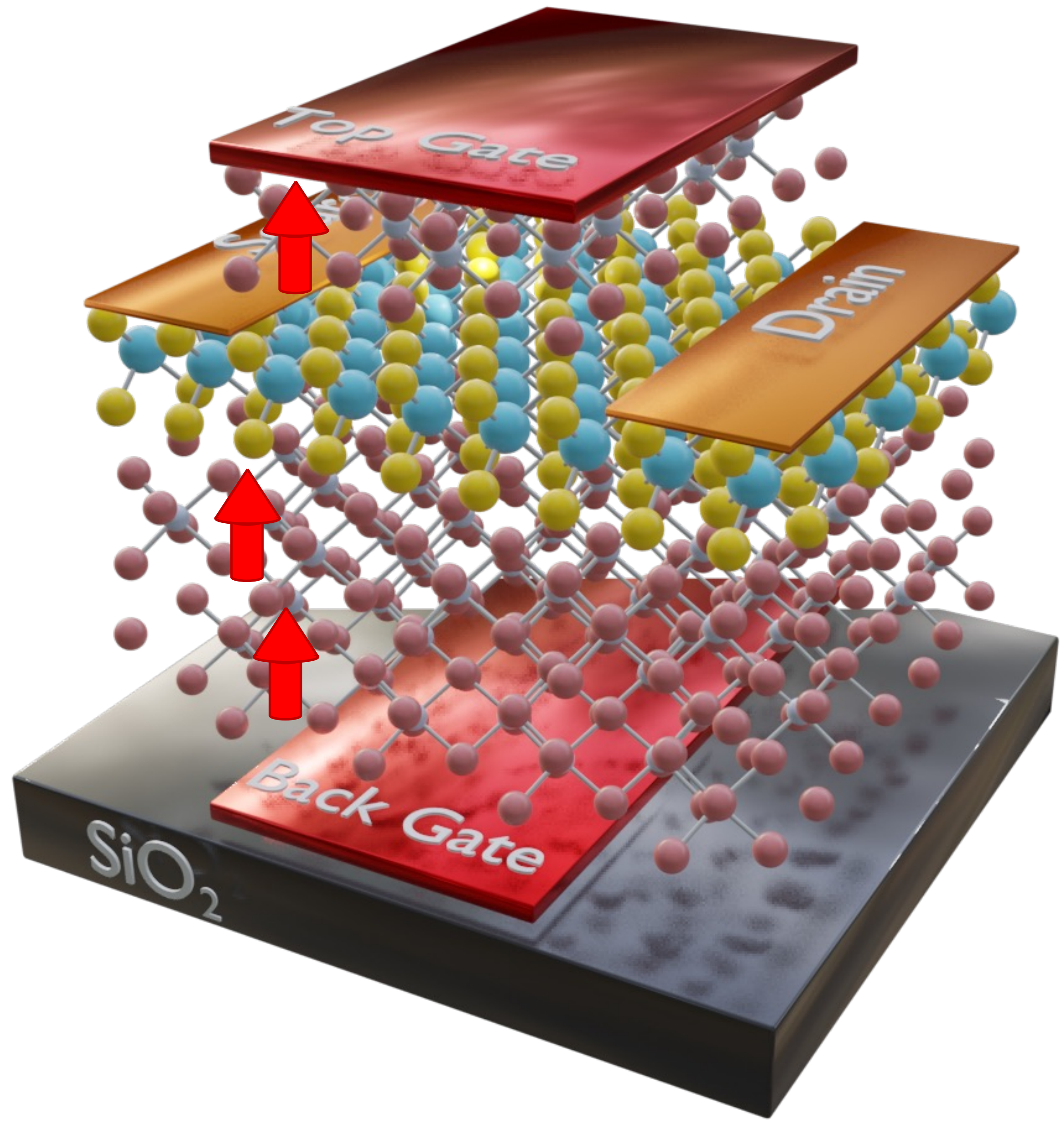
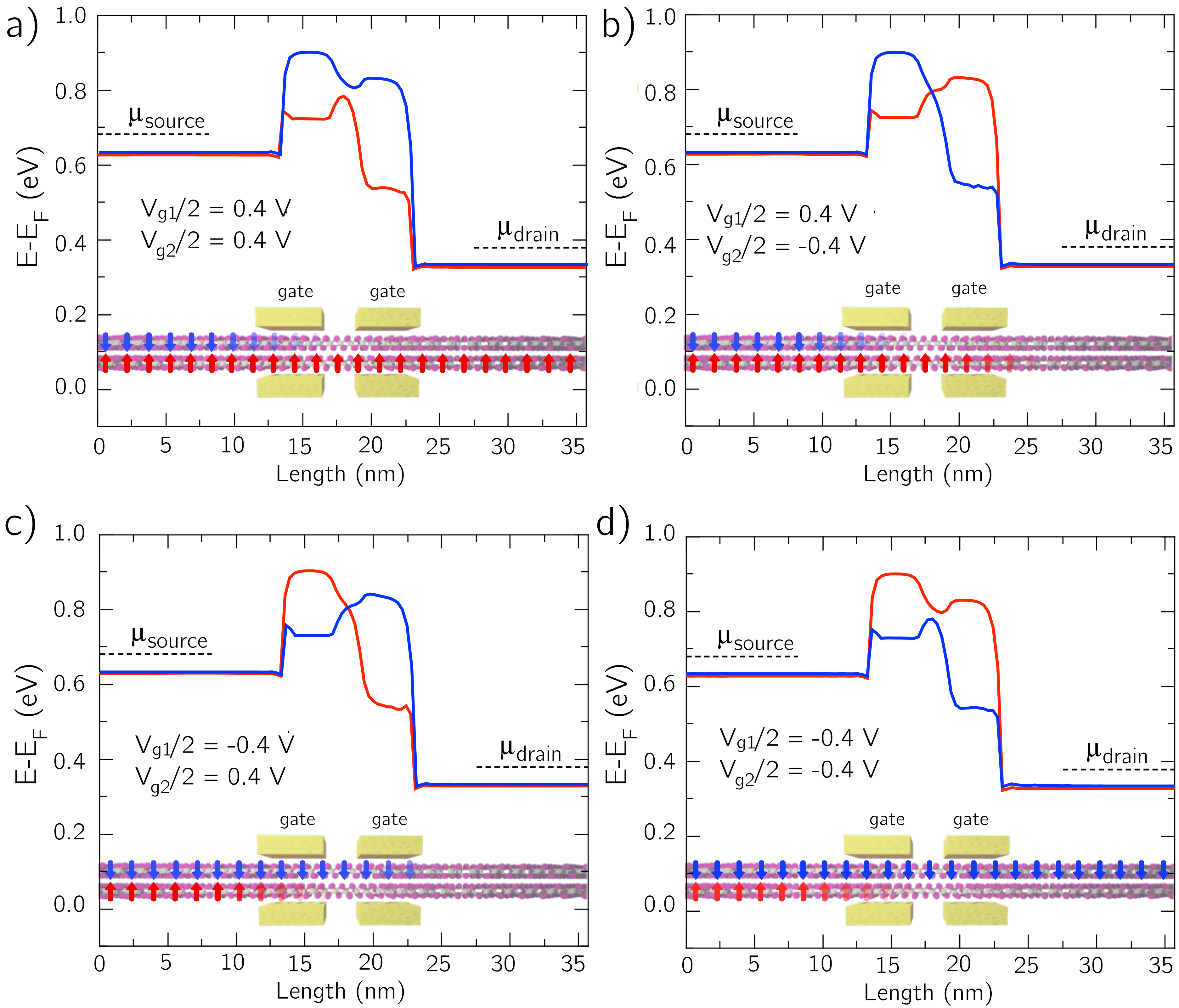
Thank you!



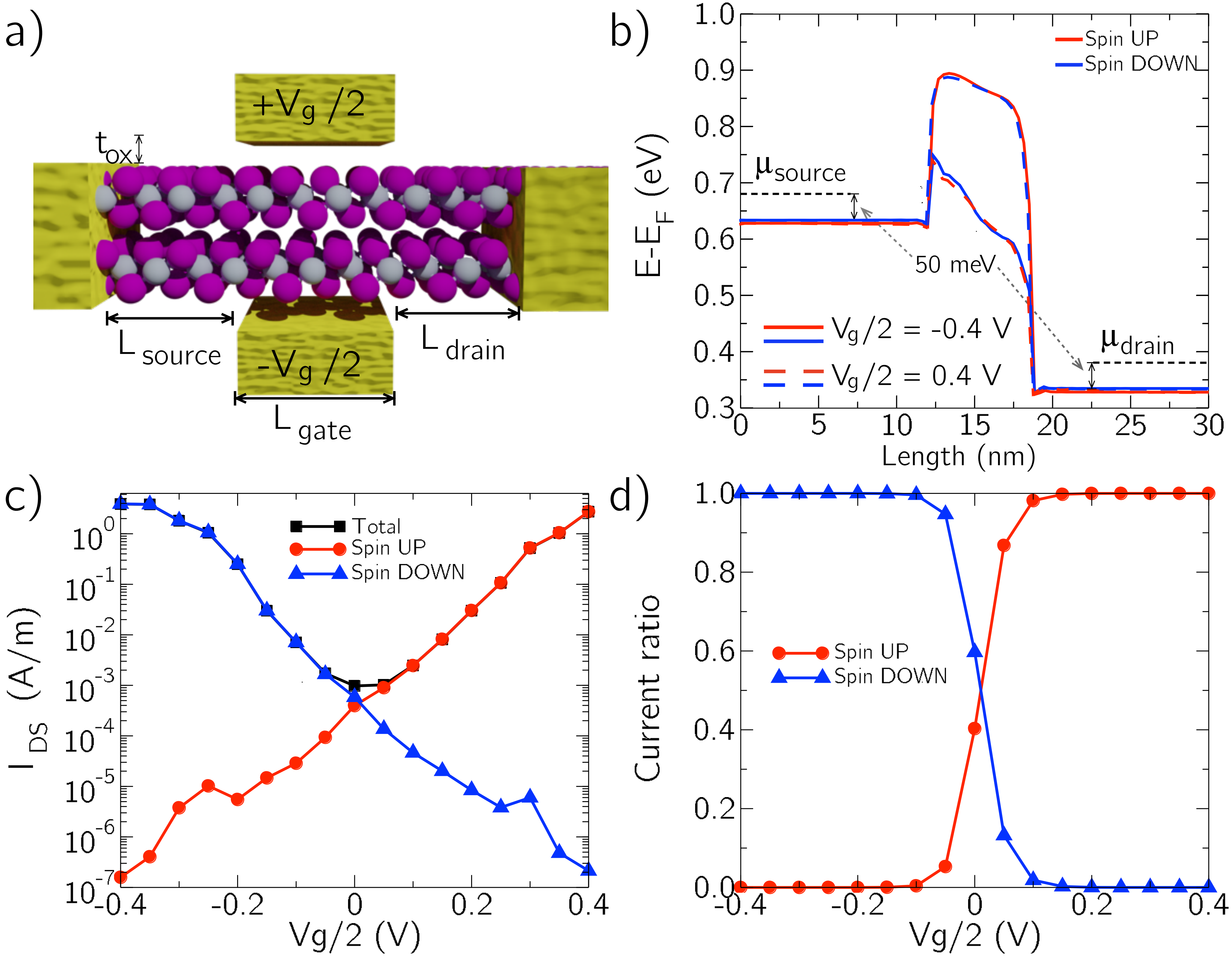
VALLEY-OFF



VALLEY-ON



a)
μ_{source}
μ_{drain}
$V_{g1}/2$ = 0.4 V
$V_{g2}/2$ = 0.4 V
gate
gate
E-E$_F$ (eV)
Length (nm)
b)
μ_{source}
μ_{drain}
$V_{g1}/2$ = 0.4 V
$V_{g2}/2$ = -0.4 V
gate
gate
E-E$_F$ (eV)
Length (nm)
c)
μ_{source}
μ_{drain}
$V_{g1}/2$ = -0.4 V
$V_{g2}/2$ = 0.4 V
gate
gate
E-E$_F$ (eV)
Length (nm)
d)
μ_{source}
μ_{drain}
$V_{g1}/2$ = -0.4 V
$V_{g2}/2$ = -0.4 V
gate
gate
E-E$_F$ (eV)
Length (nm)



a)
$+V_g/2$
t_{ox}
L_{source}
$-V_g/2$
L_{drain}
L_{gate}
b)
Spin UP
Spin DOWN
μ_{source}
50 meV
μ_{drain}
$V_g/2 = -0.4$ V
$V_g/2 = 0.4$ V
$E-E_F$ (eV)
Length (nm)
c)
Total
Spin UP
Spin DOWN
I_{DS} (A/m)
Vg/2 (V)
d)
Spin UP
Spin DOWN
Current ratio
Vg/2 (V)