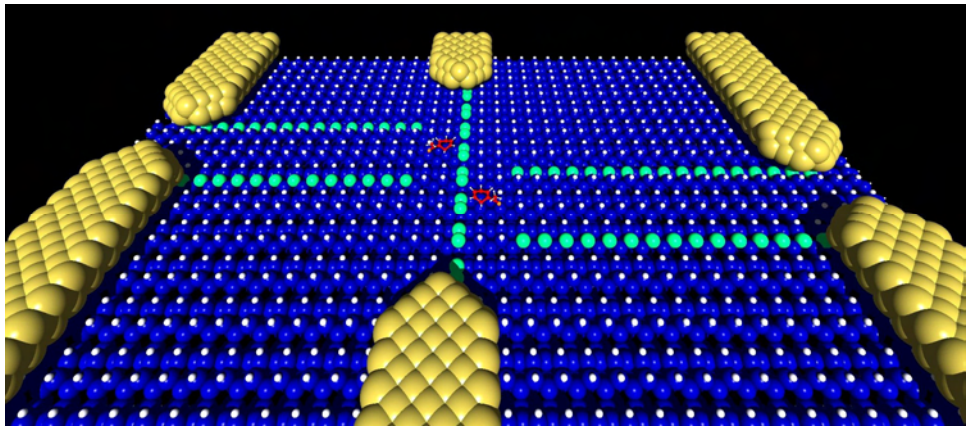
Large dangling bond electronic circuits with the supporting surface and contacting nano-pads

Francisco Ample, Hiroyo Kawai, Mark Saeys,
Kian Soon Yong, Kuan Eng Johnson Goh

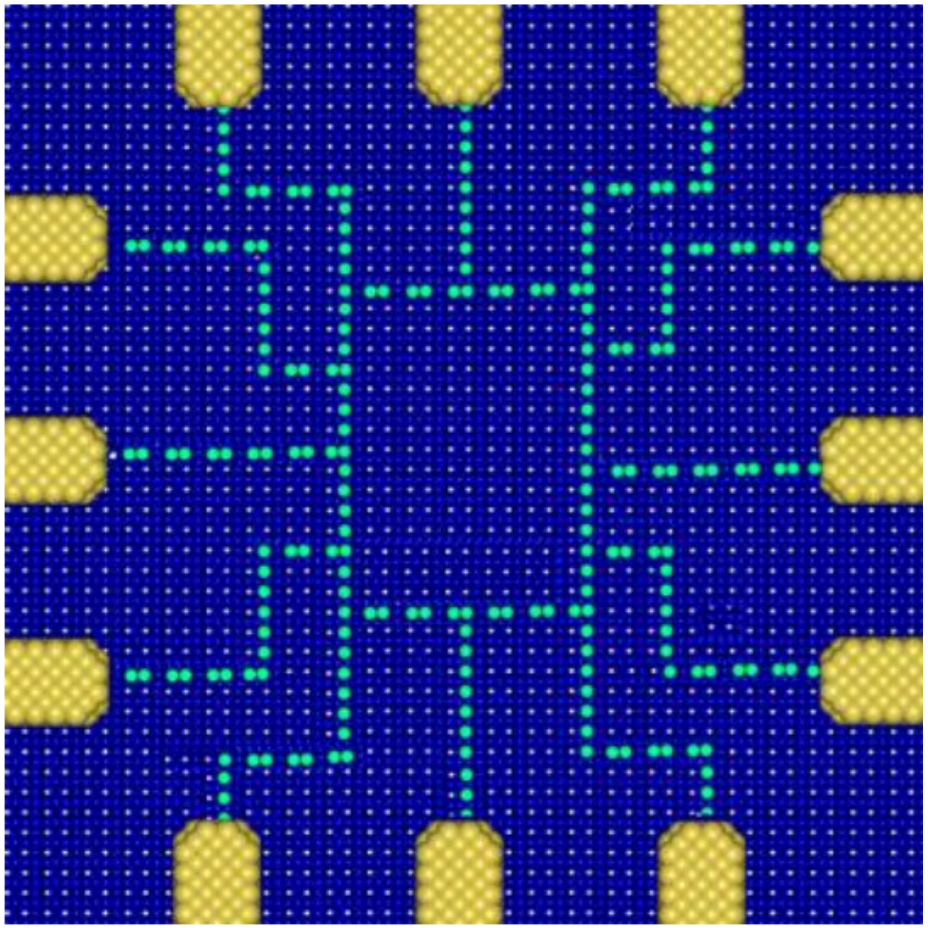


AtMol

Agency for Science, Technology and Research
SINGAPORE

OBJECTIVE

-theoretical design of atomic scale circuits



OBJECTIVE

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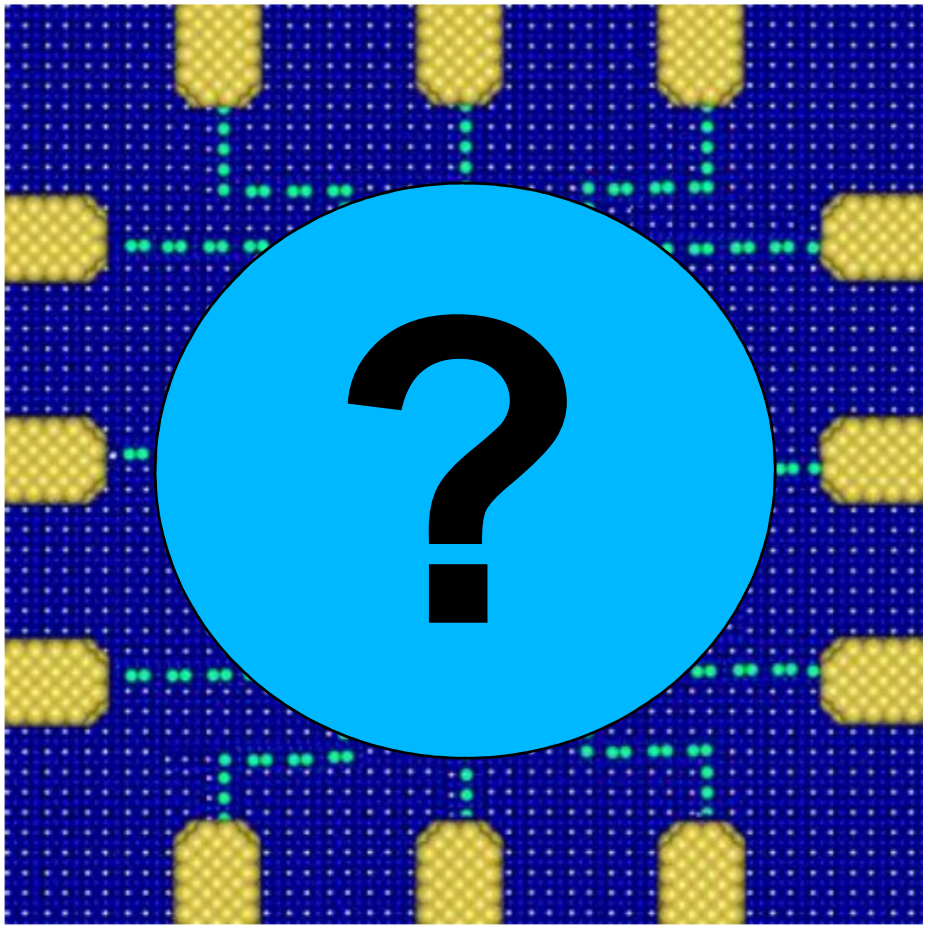
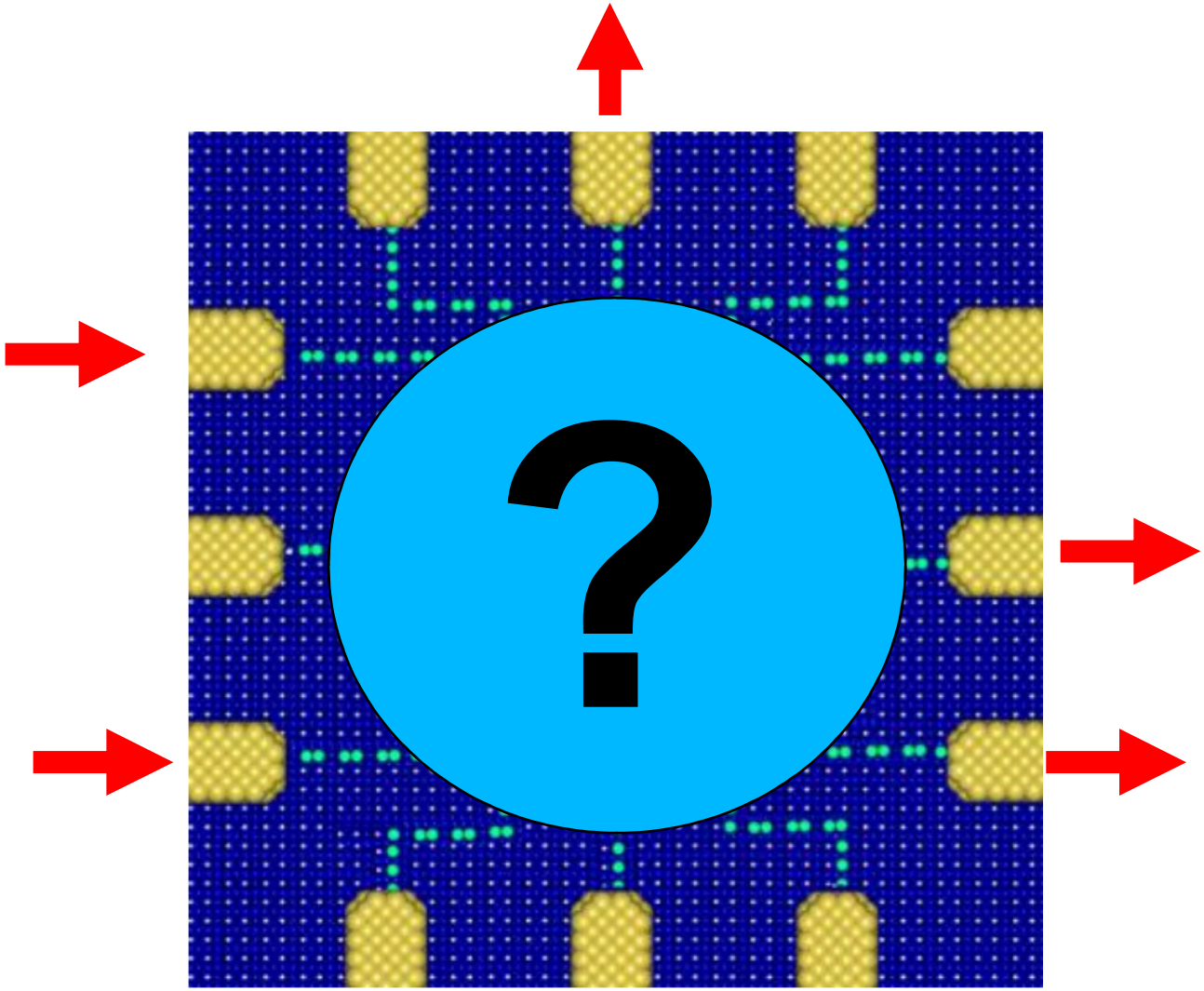
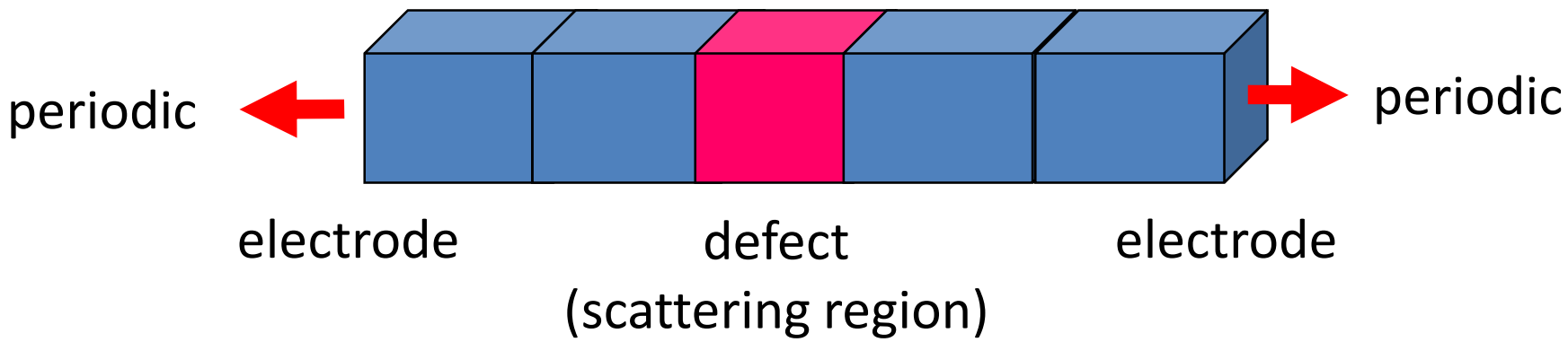




An example of a multi-channel scatering problem



Schrodinger Equation
$H\psi=E\psi$

Spatial propagator

Transfer Matrix

Spatial propagator Kernel:
Green function

=

Scattering Matrix

ESQC (Effective Hamiltonian)

Scattering Matrix

Self-Energy

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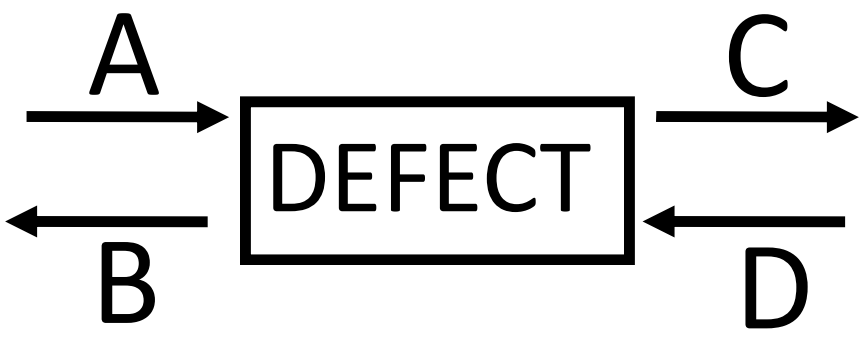
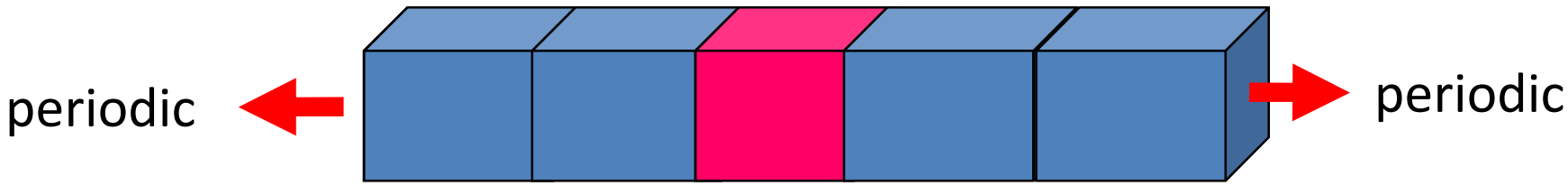


Amplitudes of the incoming
and outcoming plane waves

$$T(E)=\frac{|C|^2}{|A|^2}$$

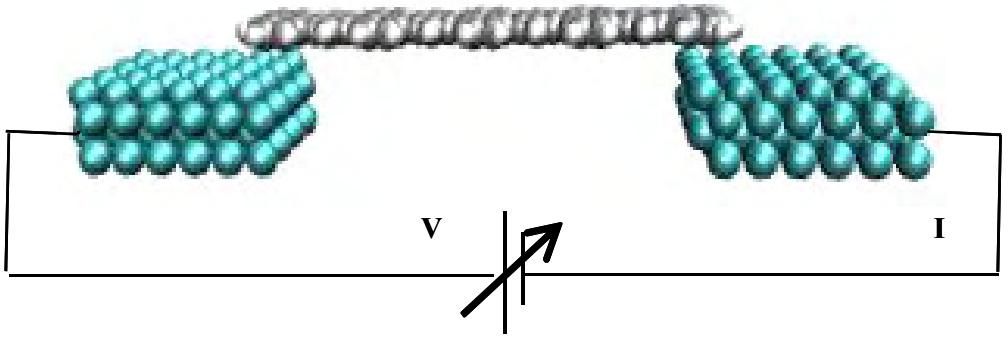
$$I(V,x,y,z)=\frac{e}{\pi\hbar}\int_{E_f}^{E_f+eV}T(E,x,y,z)\,dE$$

ESQC



electrode defect electrode

(scattering region)

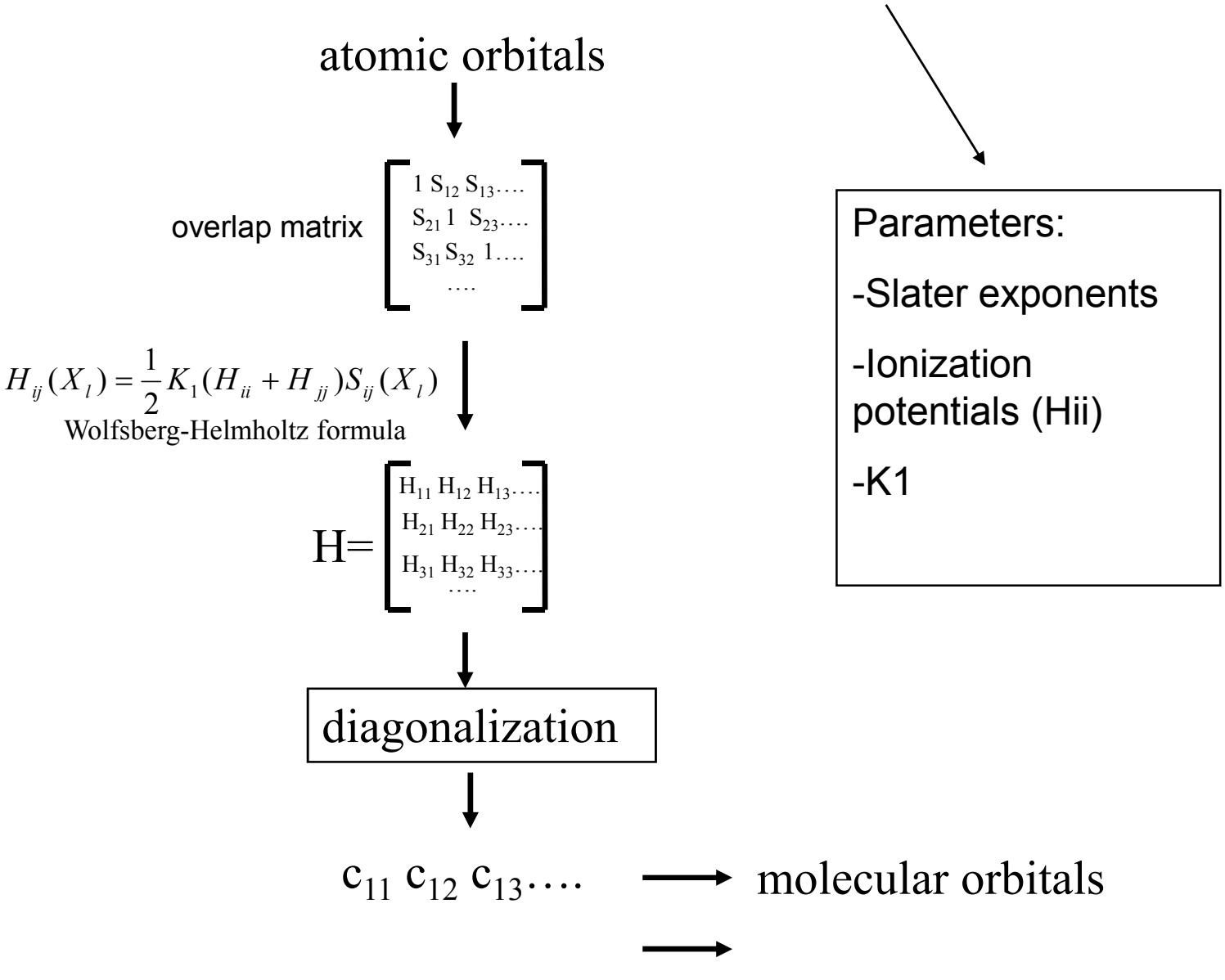


Extended Huckel MO aproximation:

-parameters are fitted with comparison with DFT calculations

P. Sautet and C. Joachim, Phys. Rev. B 38 (1988) 12238

LCAO Basis set + DFT fitting

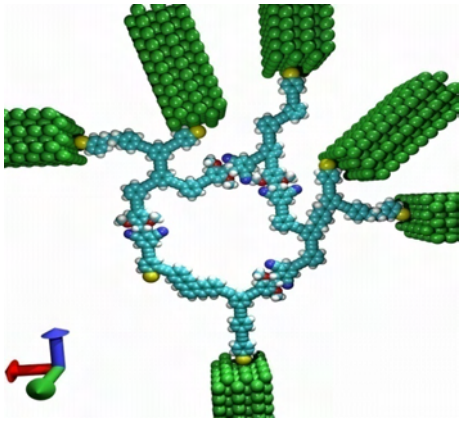


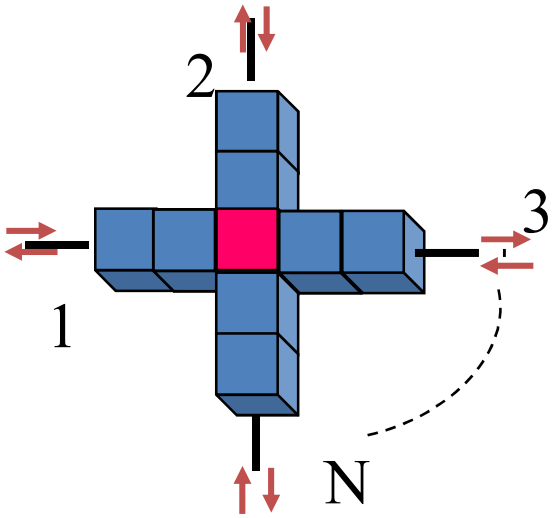
N-ESQC

-electron transport calculations of atomic scale circuits driven in a ballistic or tunneling regime + the supporting surface

-Elastic Scattering Quantum Chemistry technique

-full scaterring matrix for N electrodes





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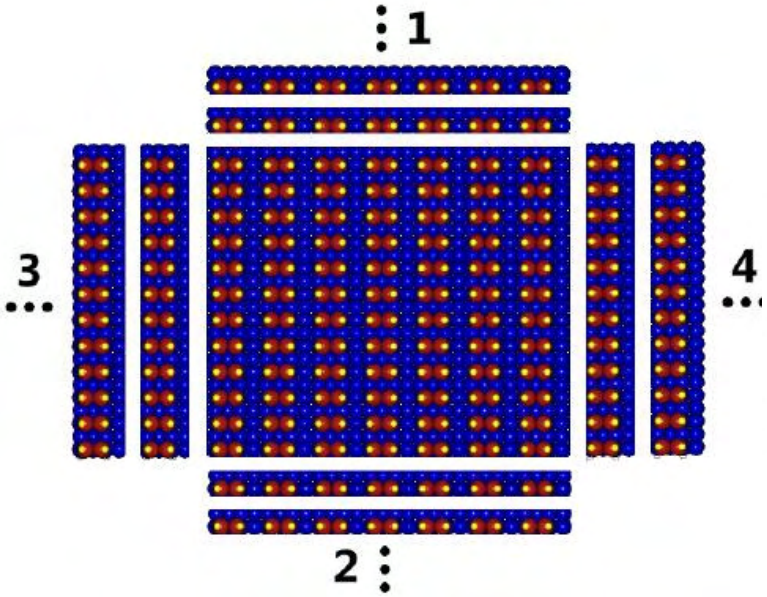
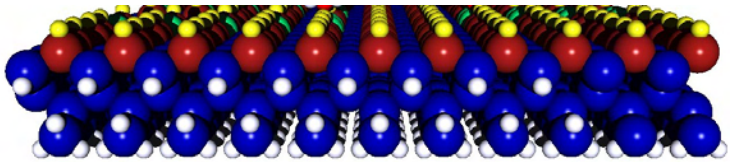
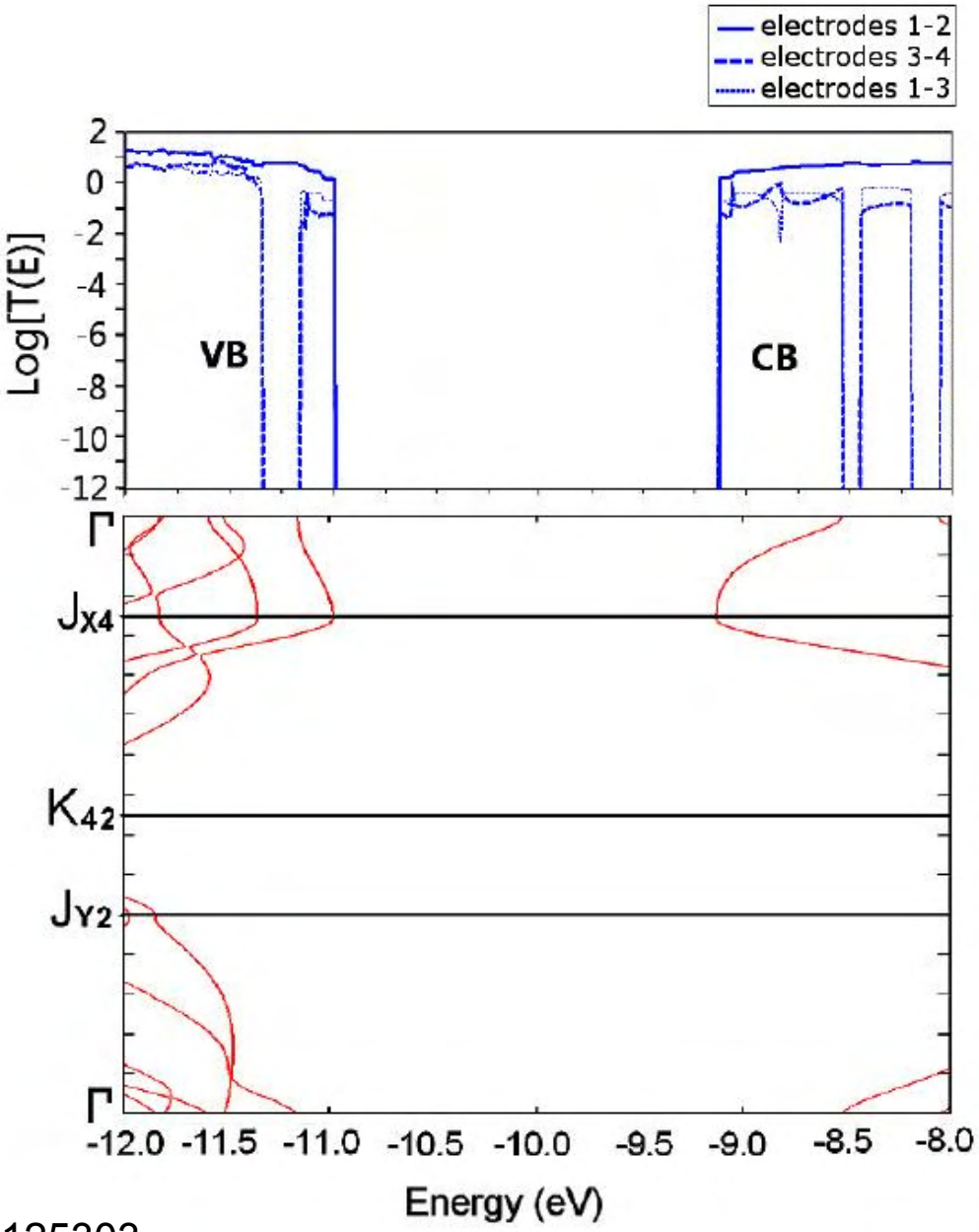
S. Ami and C. Joachim, Phys. Rev. B 65 (2002) 155419



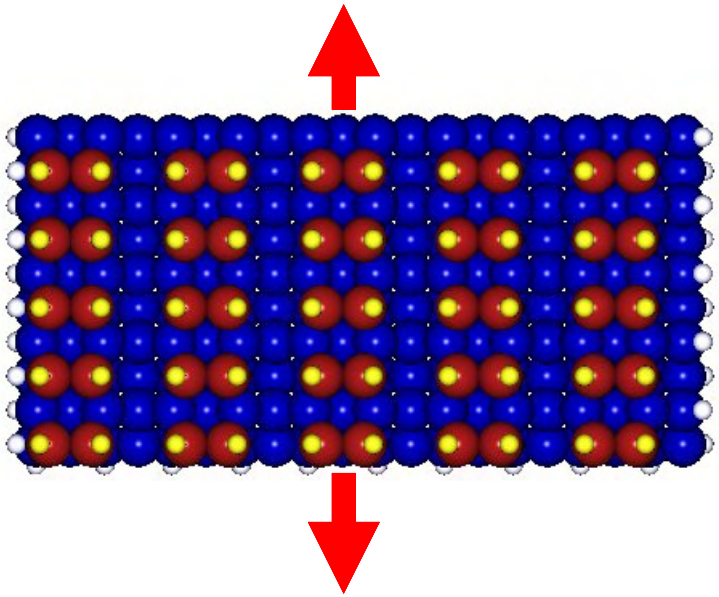
3696 atoms

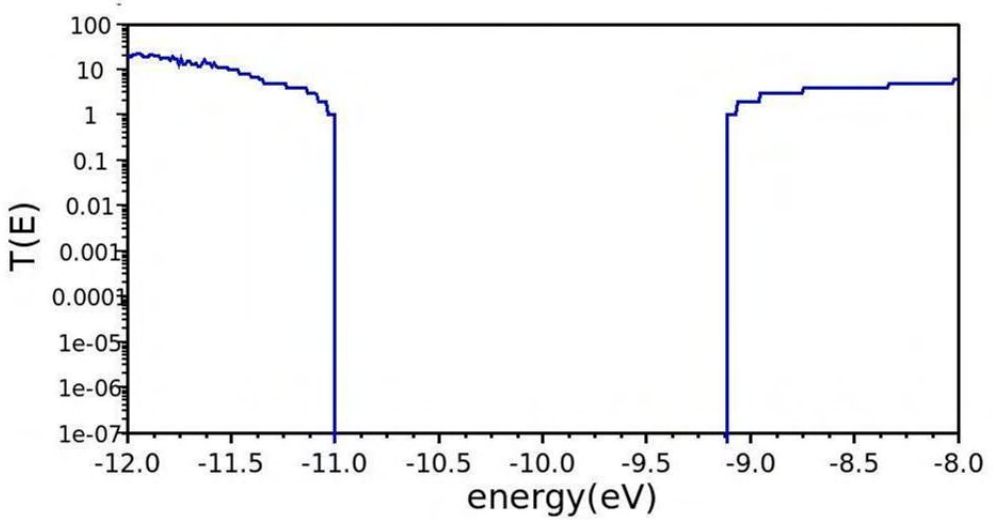




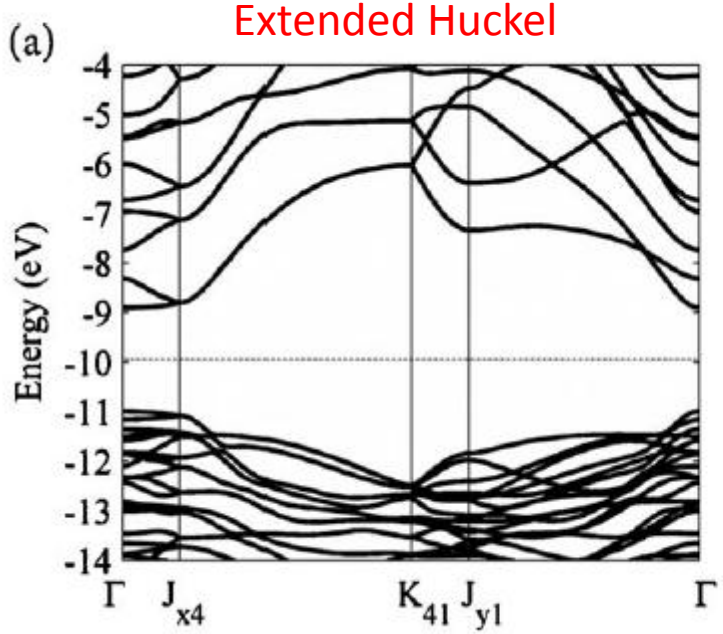
F. Ample et al, J. Phys. CM, 23 (2011) 125303

Si(001)H

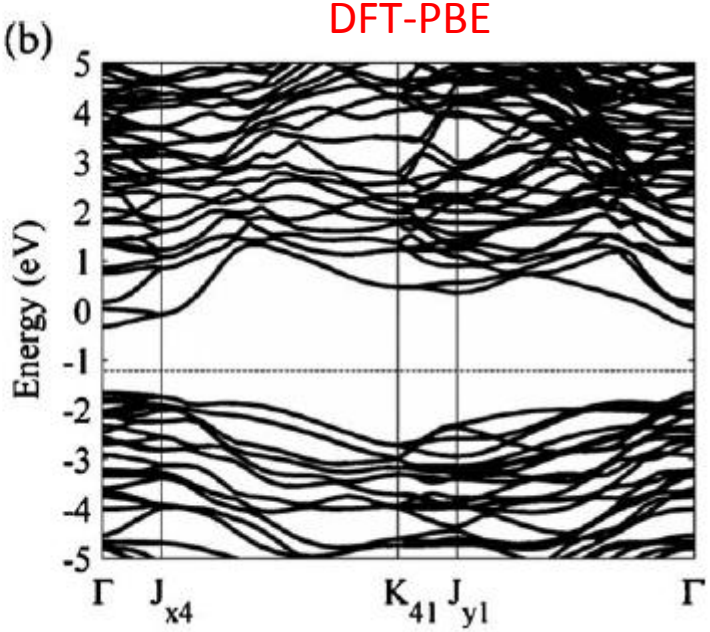




Extended Huckel

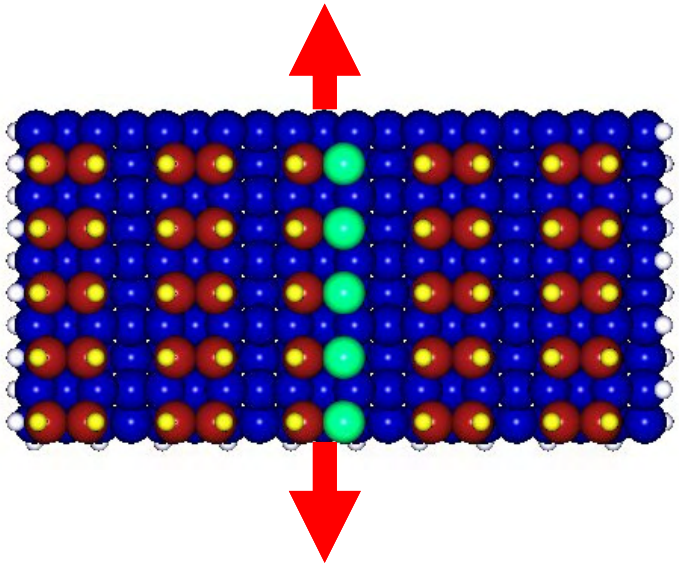


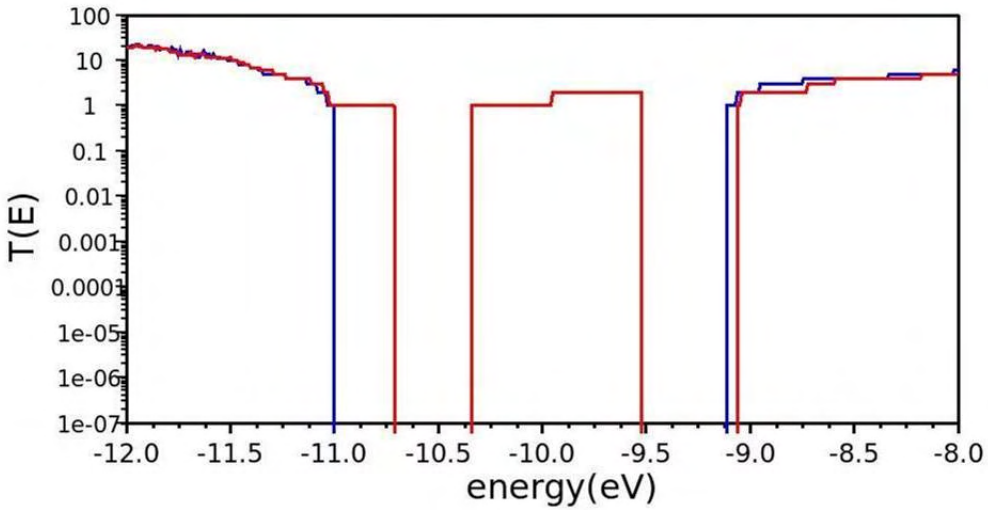
DFT-PBE



H. Kawai, Y. K. Yeo, M. Saeys and C. Joachim, Phys. Rev. B 81 (2010) 195316

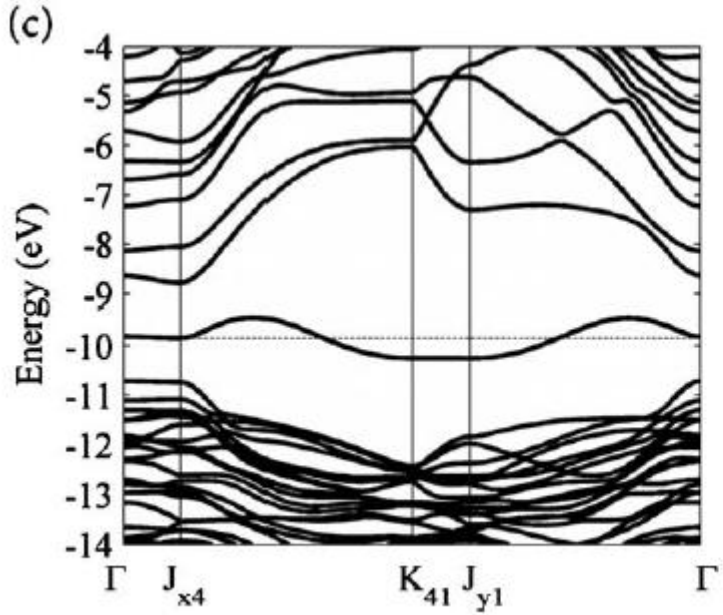
Si(001)H + dangling wire

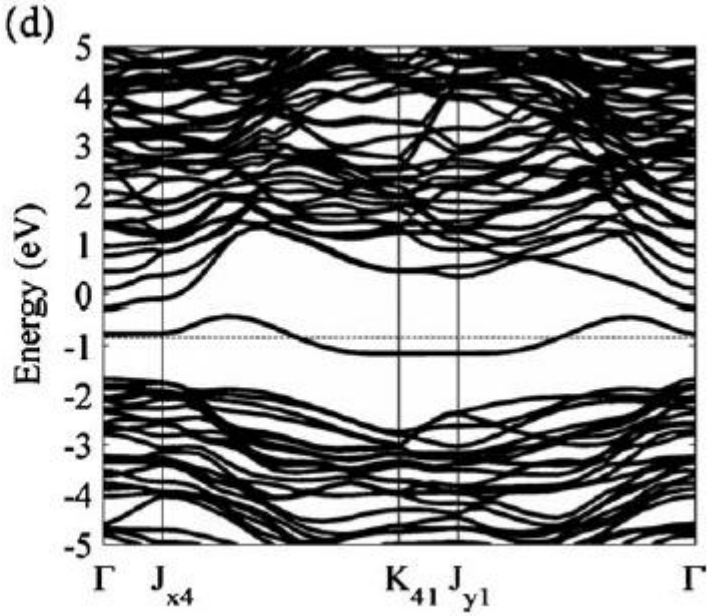




Extended Huckel

DFT-PBE





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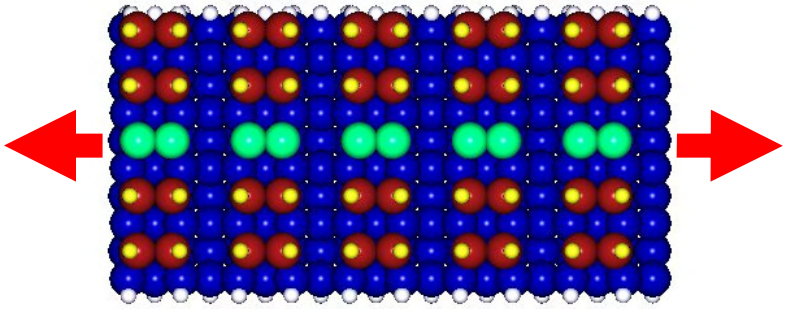
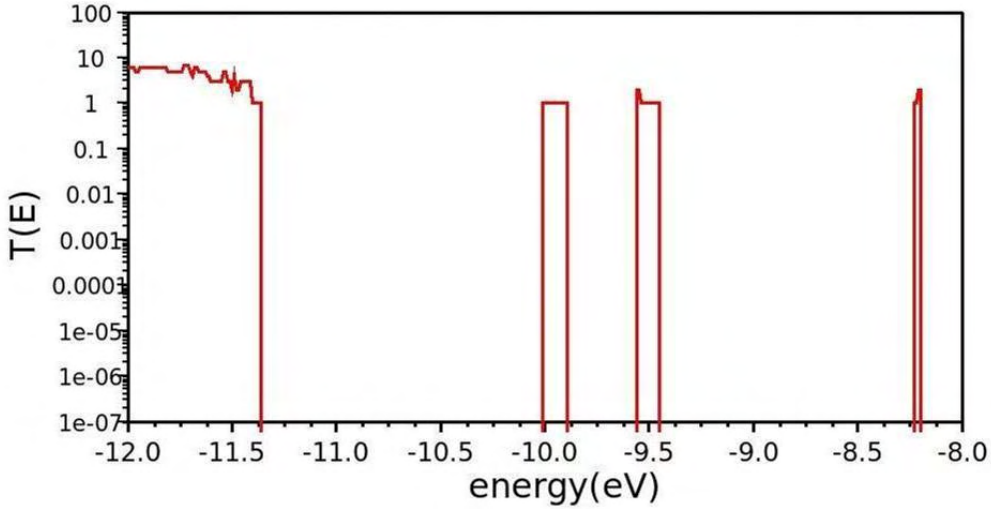
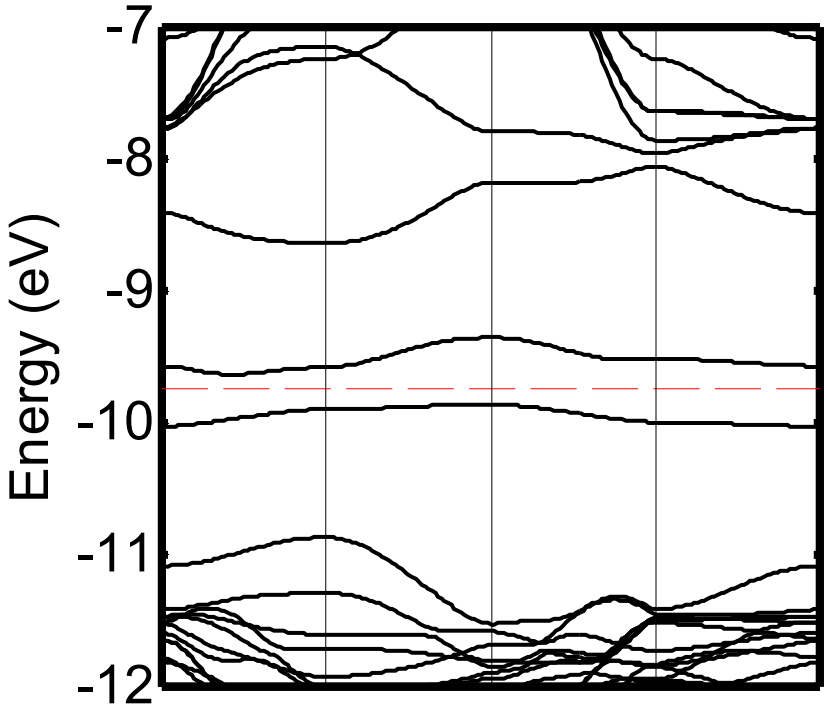


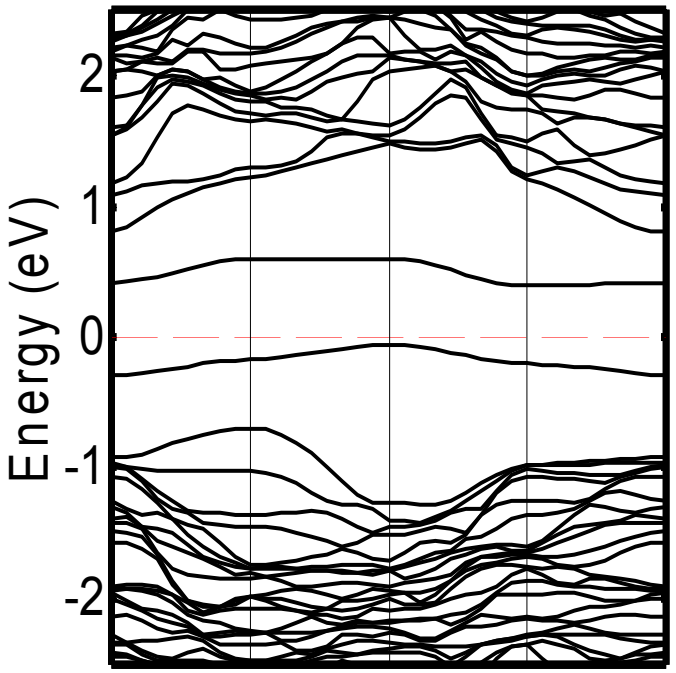


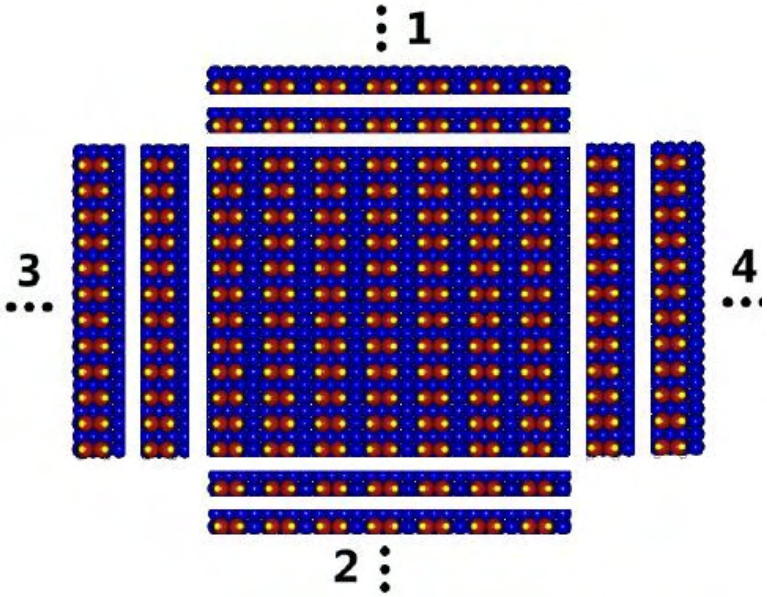
Extended Huckel



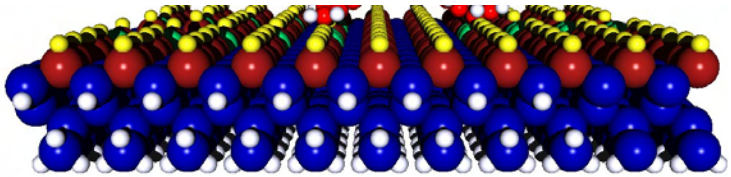
DFT-PBE

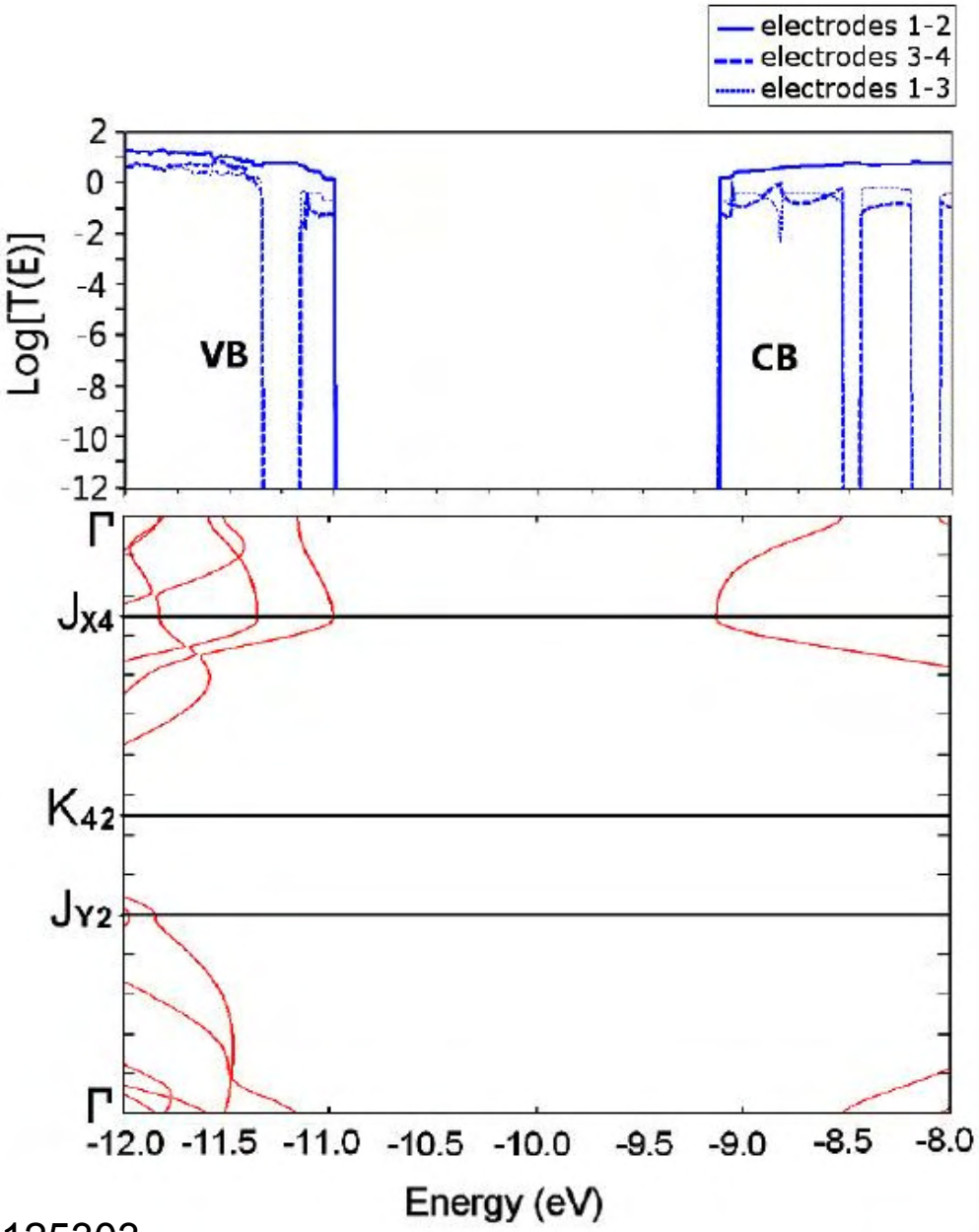
Si100H DBwperp sym 1x4 optd band



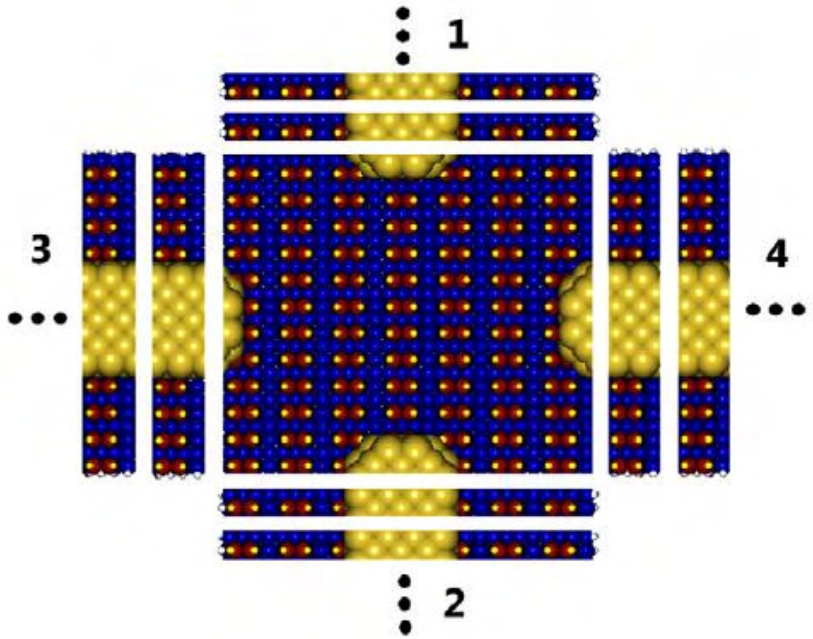


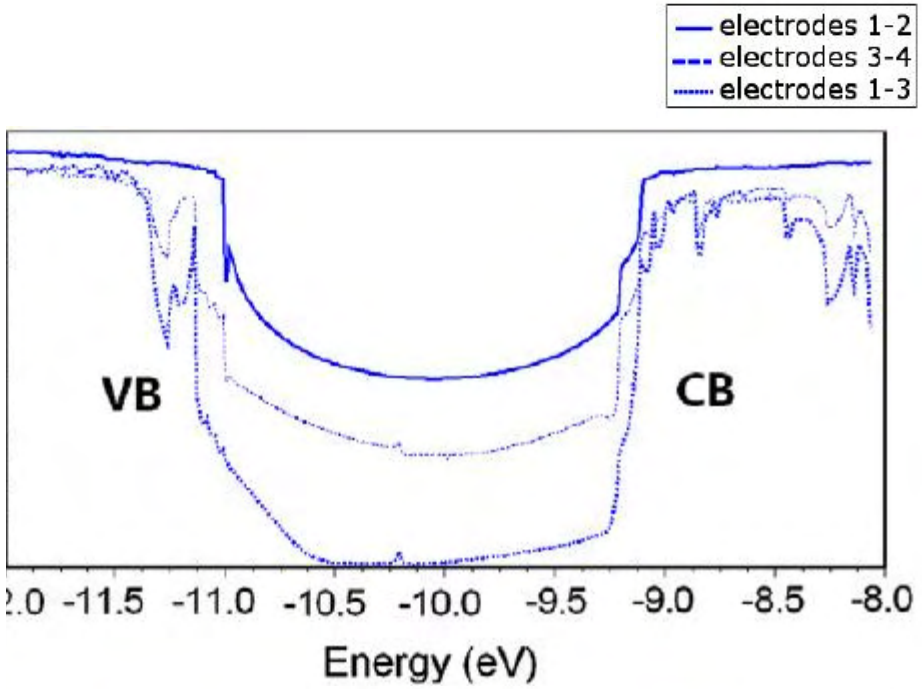
3696 atoms

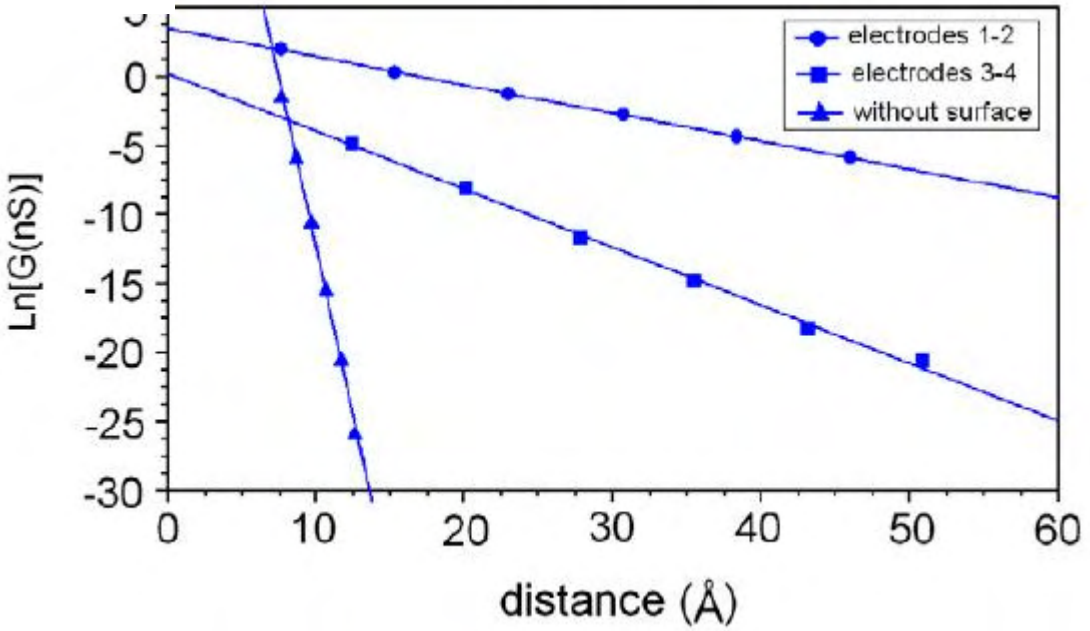




F. Ample et al, J. Phys. CM, 23 (2011) 125303







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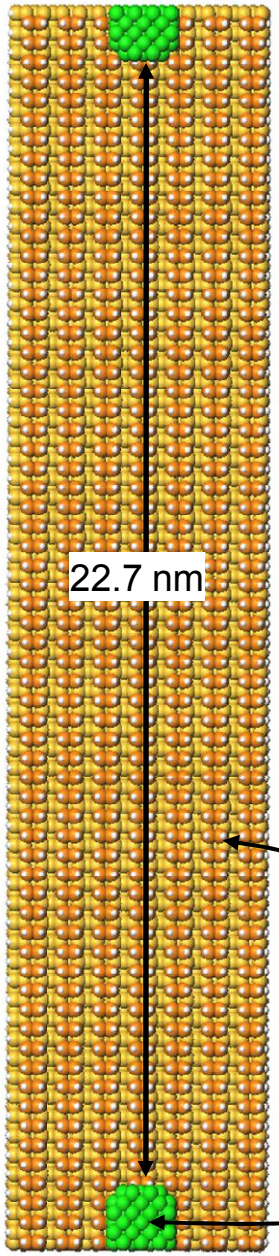
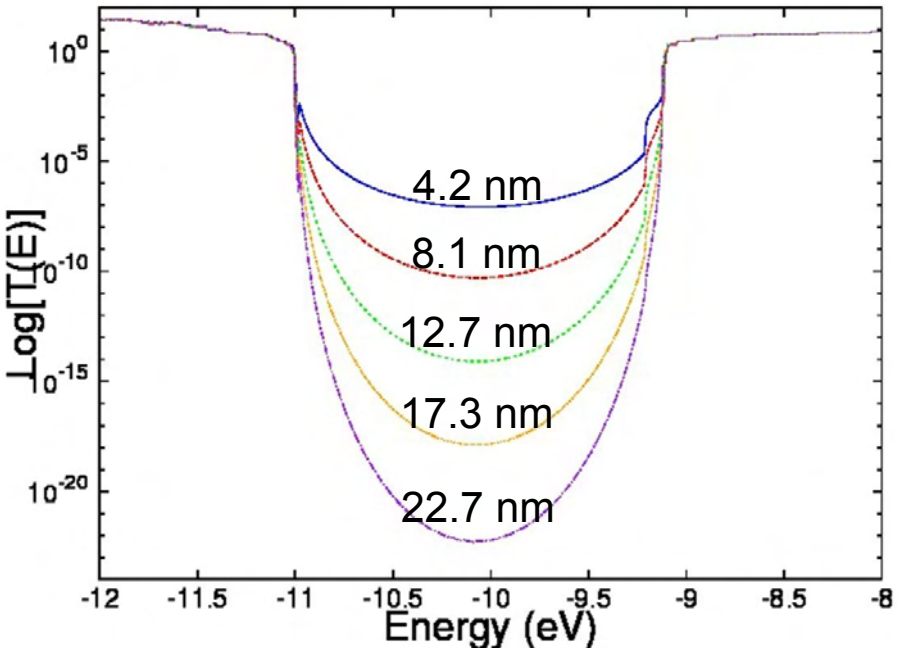
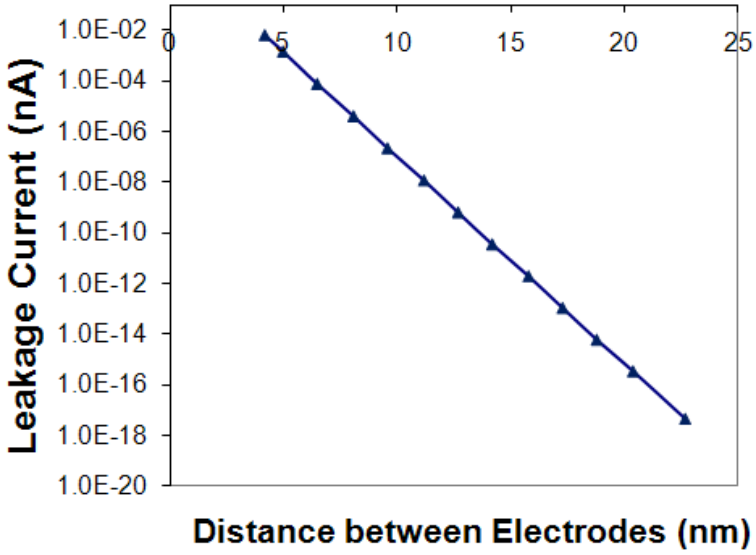
T(E) and leakage current with different inter-electrode distance on Si(100)

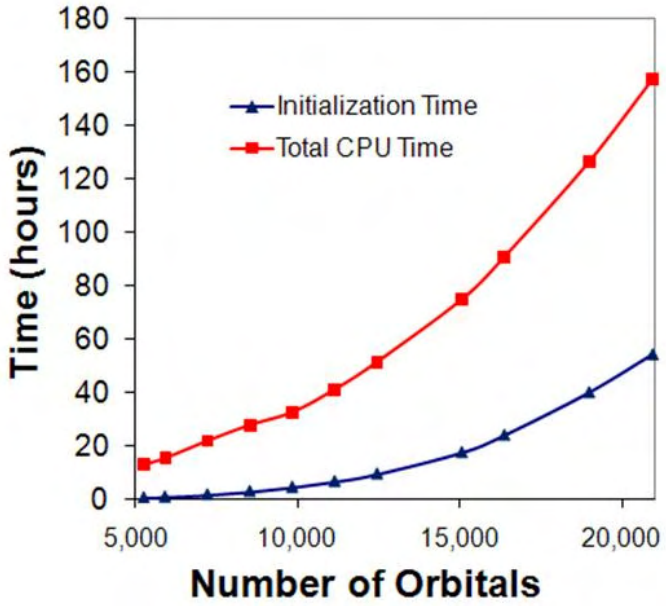


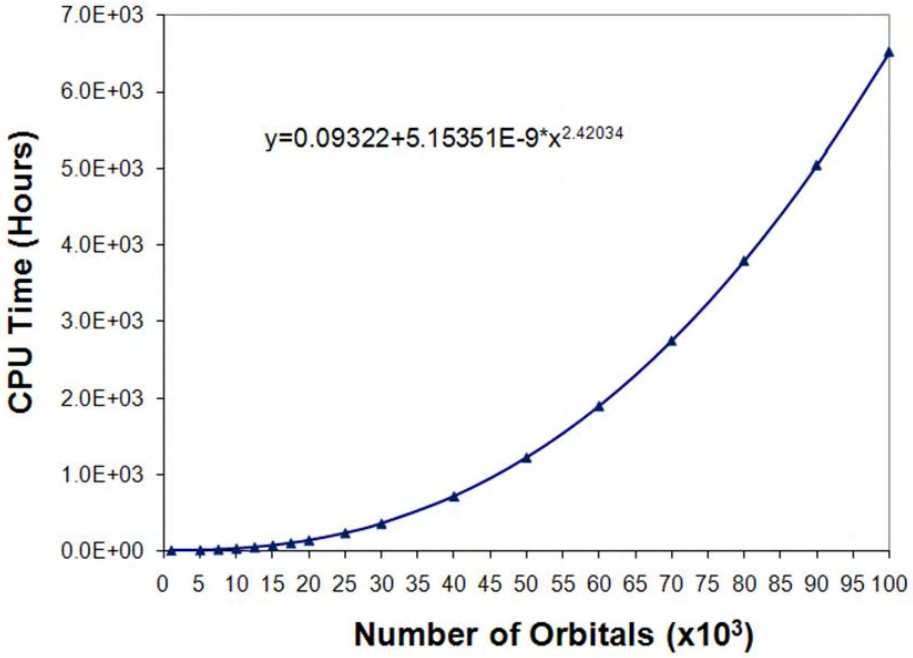


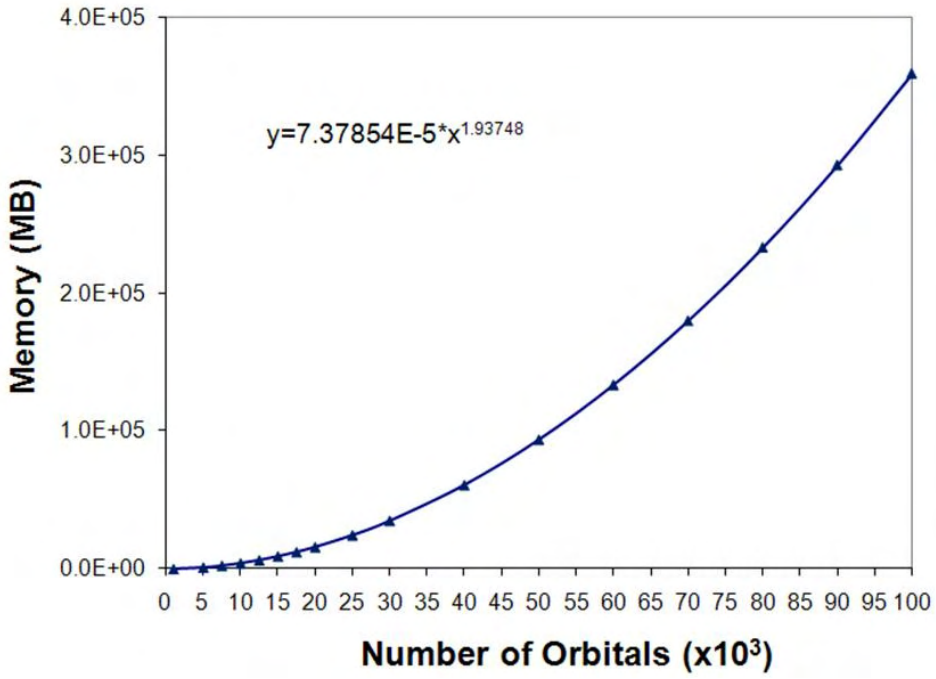


Fitted curves for CPU time and memory vs orbital number

Inter-Au Distance (nm)	Orbitals #
4.2	5289
8.1	8549
12.7	12461
17.3	16373
22.7	20937

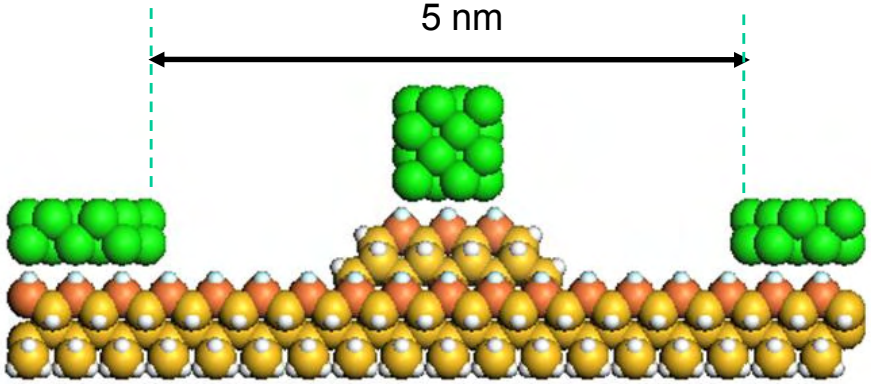


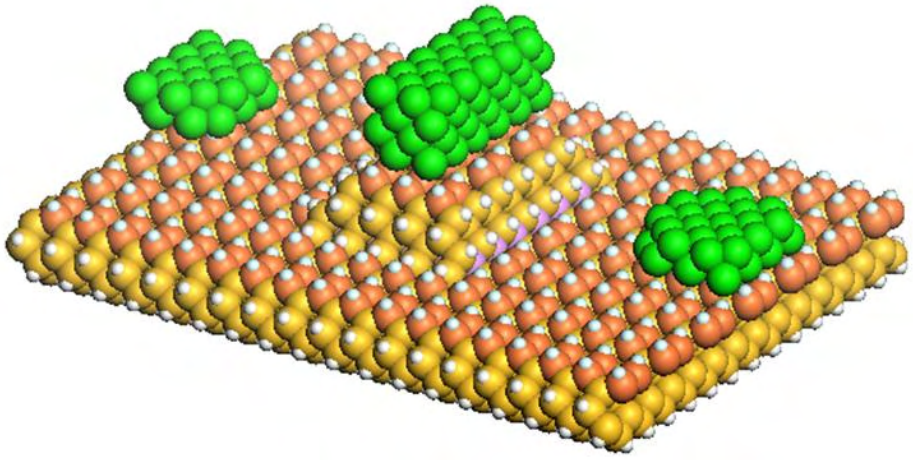




Scalling down the transistor down to the atomic scale ?

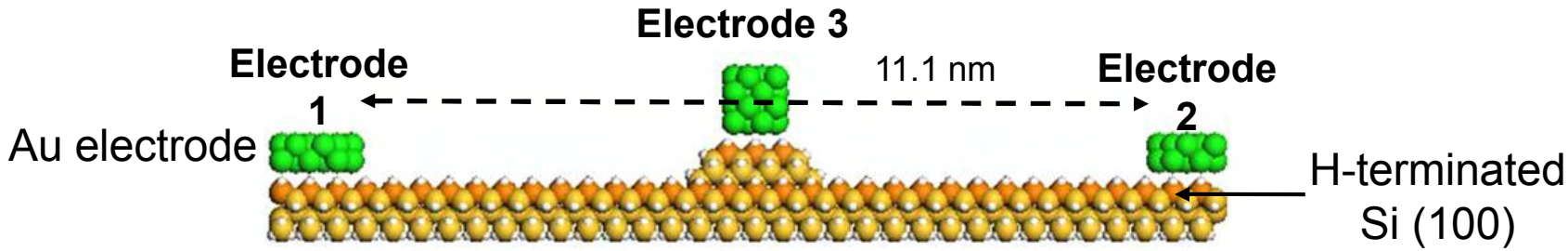
3-terminals device to emulate a transistor



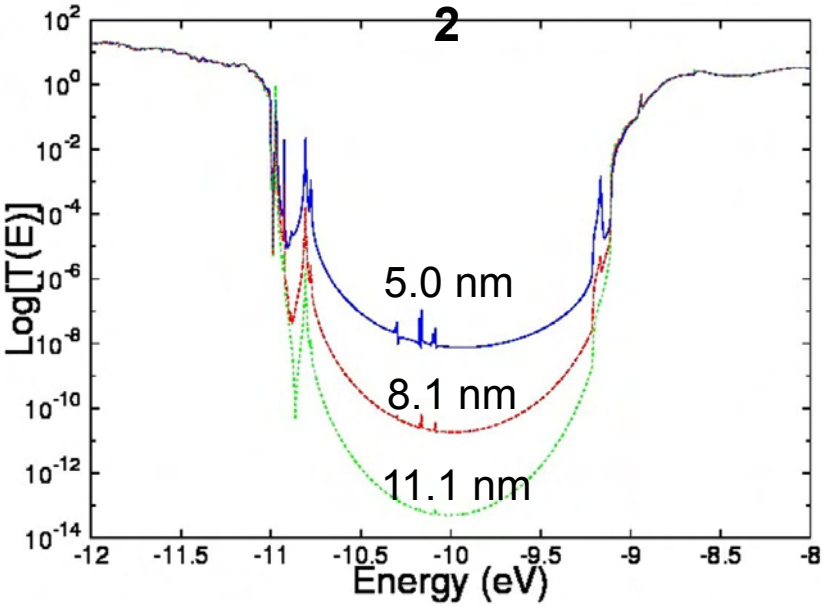


Total number of orbitals: 6351

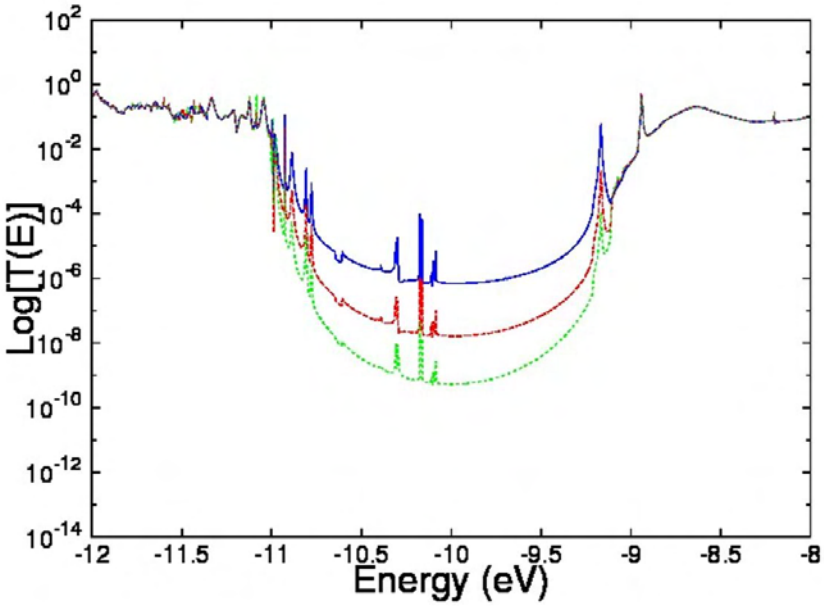
3-terminals structures that resemble transistors



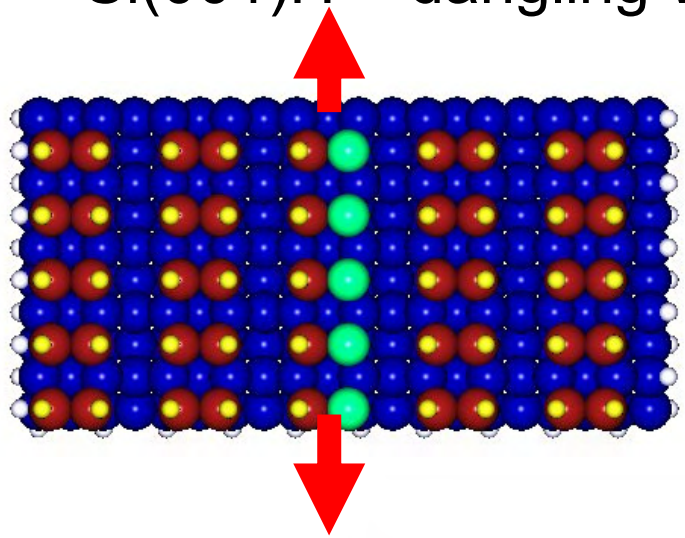
Electrodes 1-2

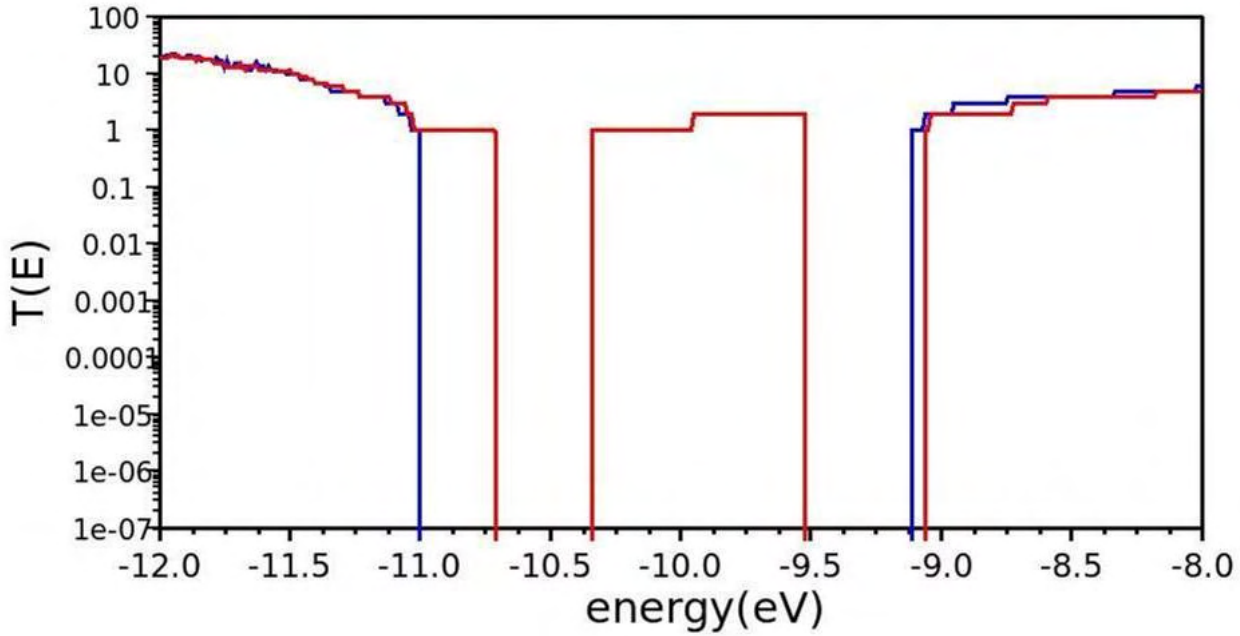


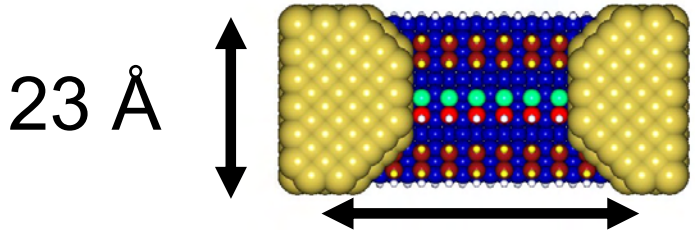
Electrodes 1-3 & 2-3



Si(001)H + dangling wire

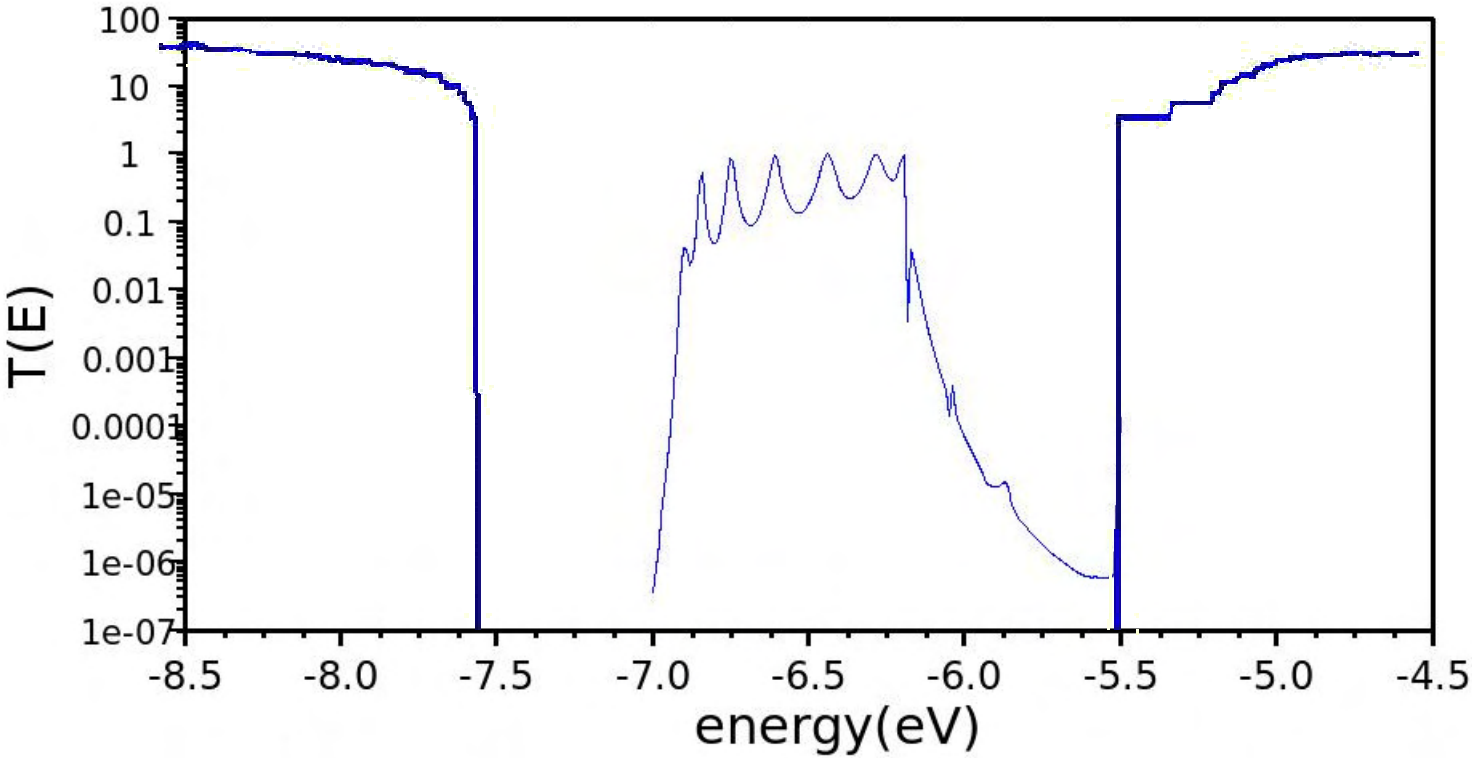


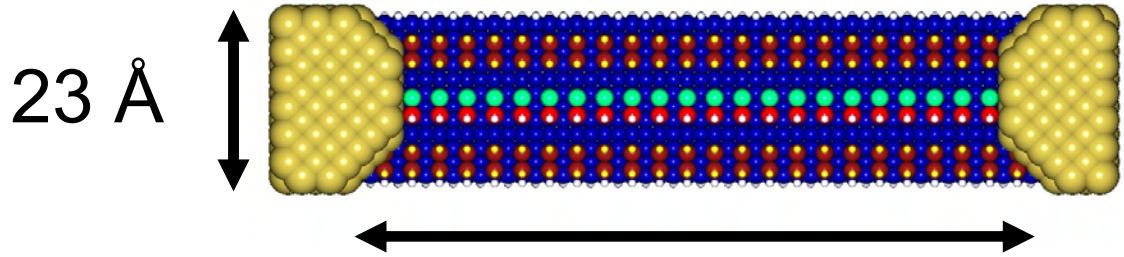


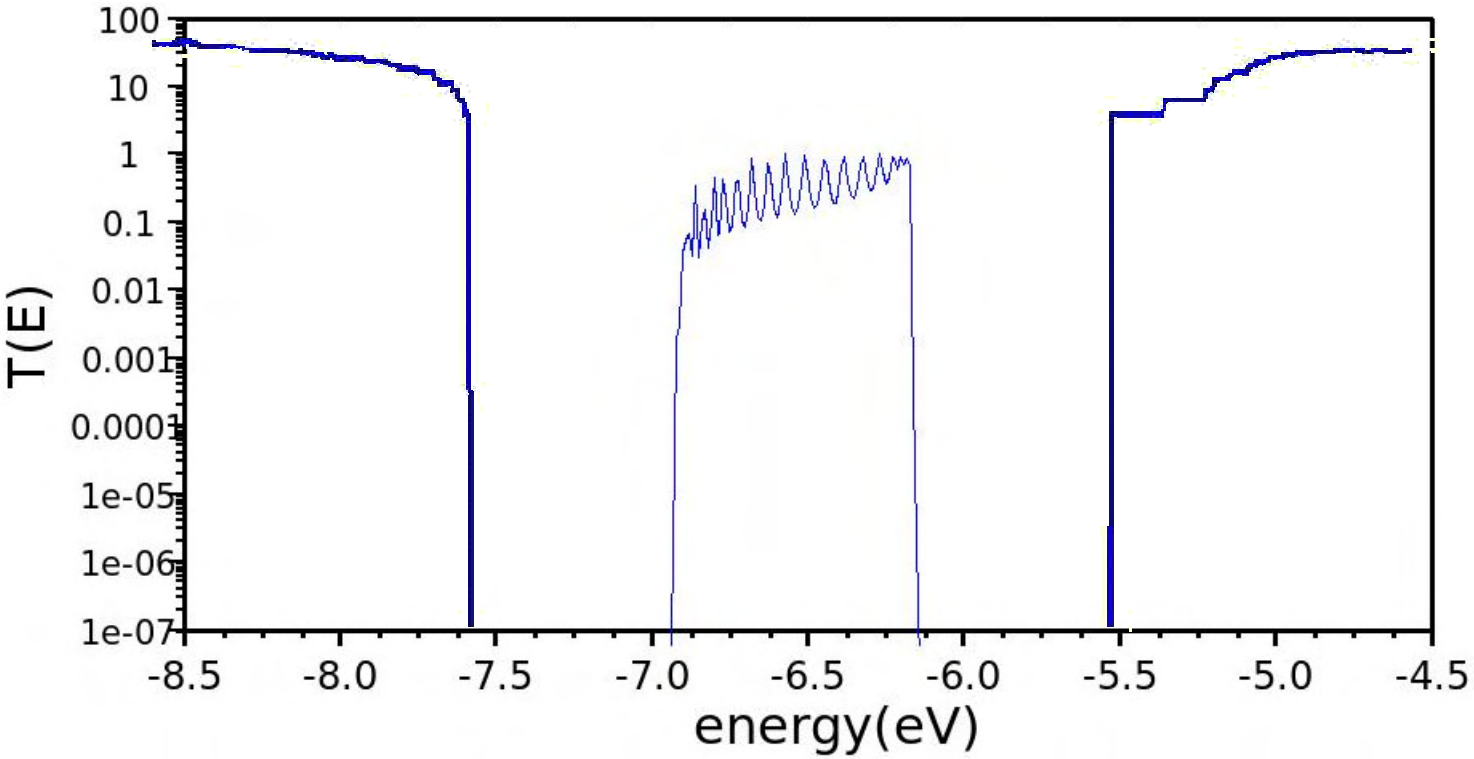


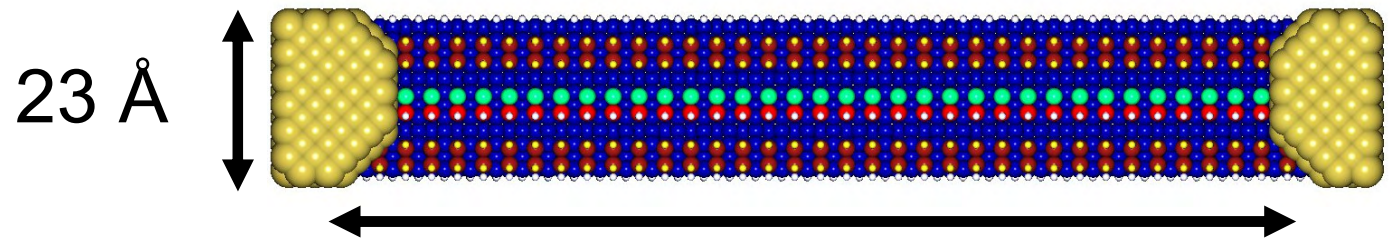
38 Å

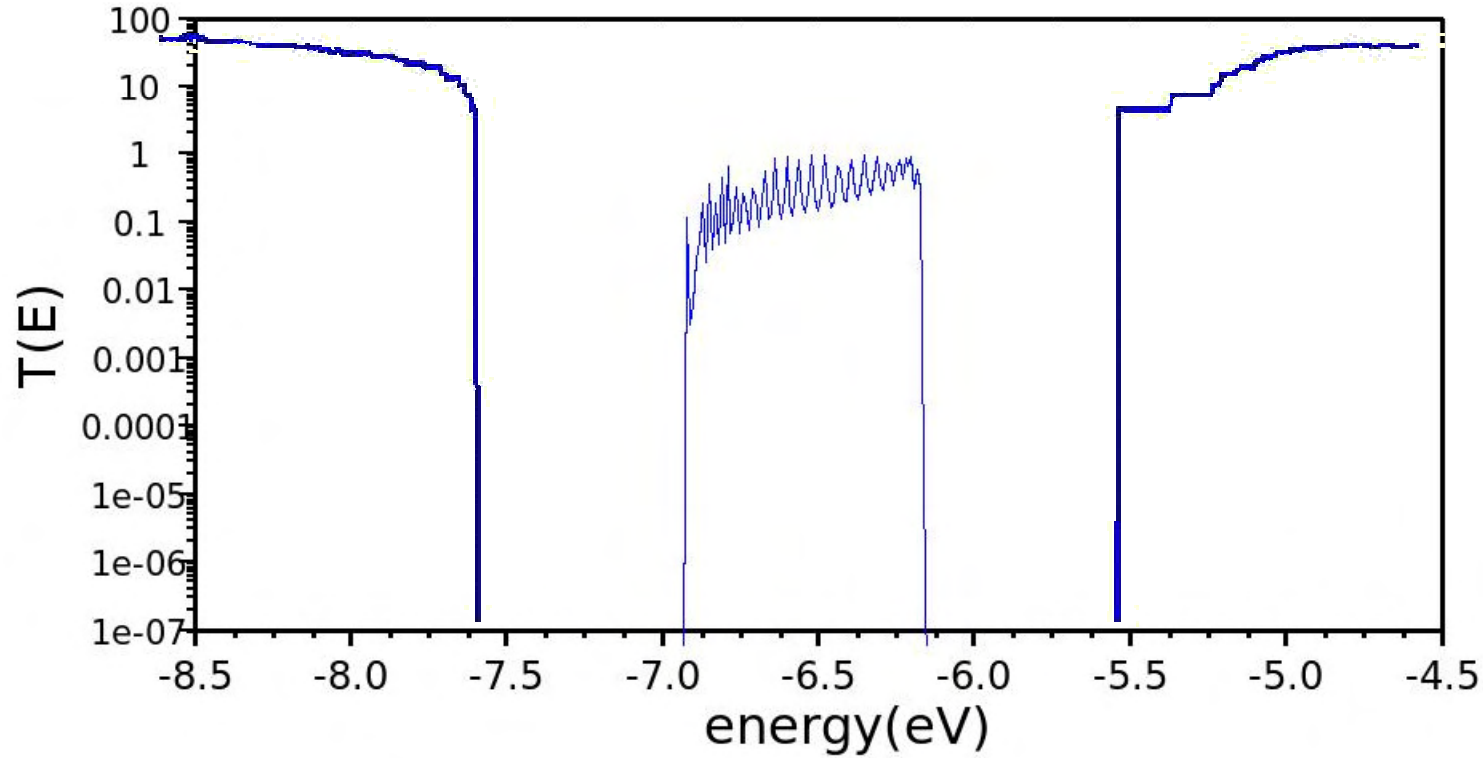
1070 atoms



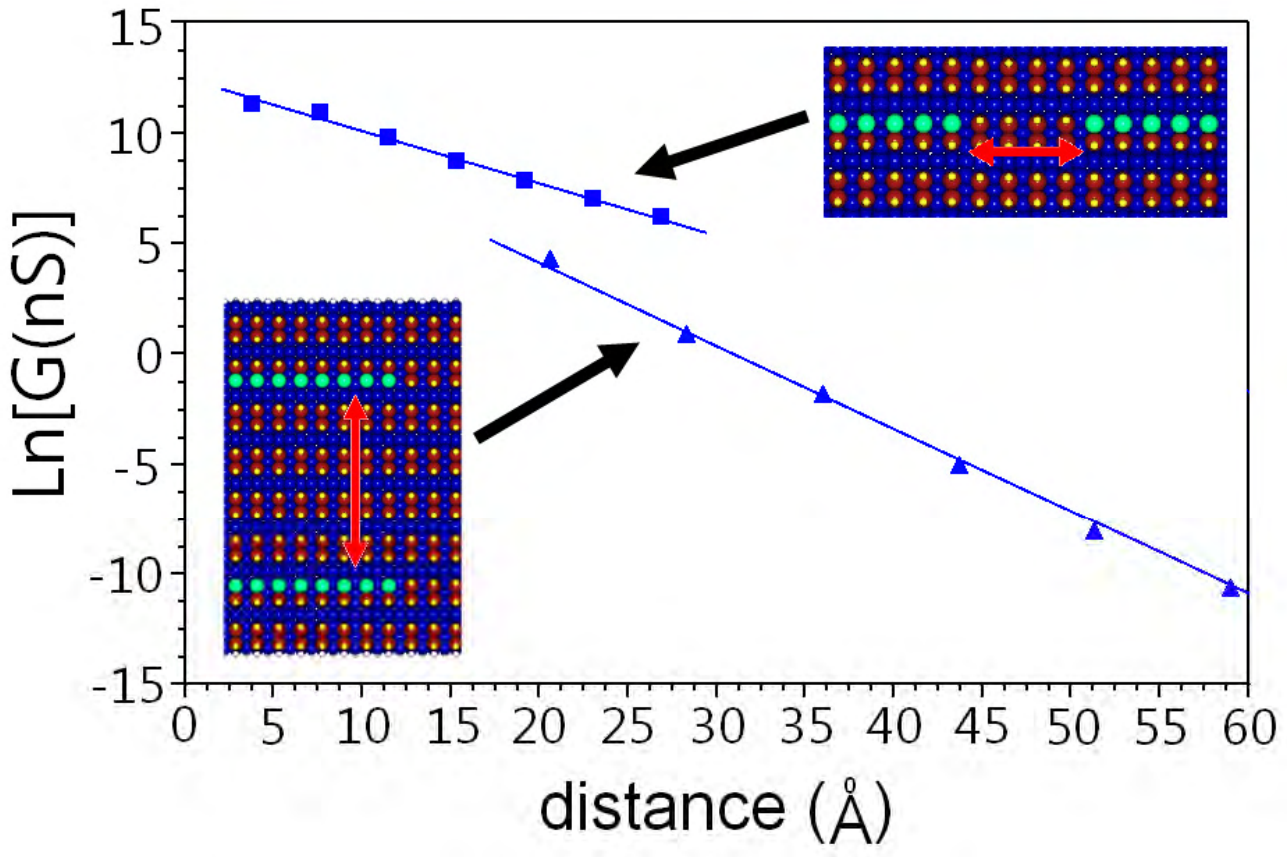

23 Å
100 Å
2142 atoms


T(E)
100
10
1
0.1
0.01
0.001
0.0001
1e-05
1e-06
1e-07
-8.5
-8.0
-7.5
-7.0
-6.5
-6.0
-5.5
-5.0
-4.5
energy(eV)


23 Å
146 Å
2946 atoms


T(E)
100
10
1
0.1
0.01
0.001
0.0001
1e-05
1e-06
1e-07
-8.5
-8.0
-7.5
-7.0
-6.5
-6.0
-5.5
-5.0
-4.5
energy(eV)

-Theoretical optimization of surface circuits on passivated semiconductors

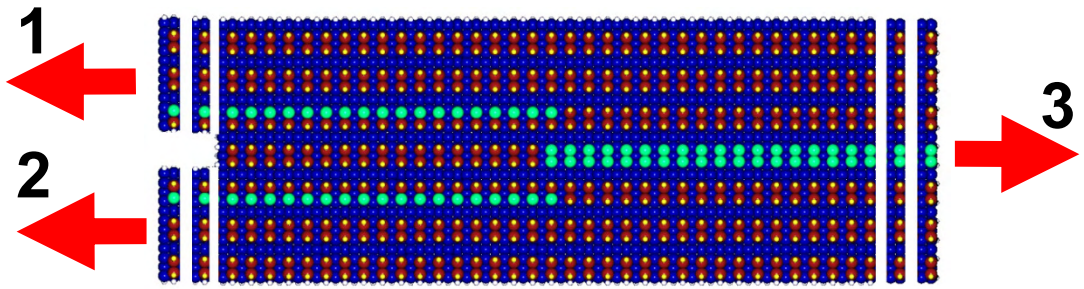


-electrons can tunnel through the surface between two separated atomic wires

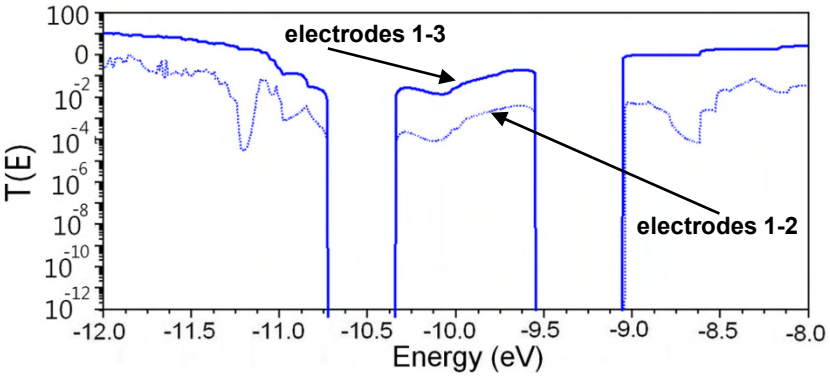
-as a tunnelling process, the conductace decay exponentially with the distance

F. Ample, I. Duchemin, M. Hliwa, C. Joachim, J. Phys. Conds. Matt. 23 (2011) 125303

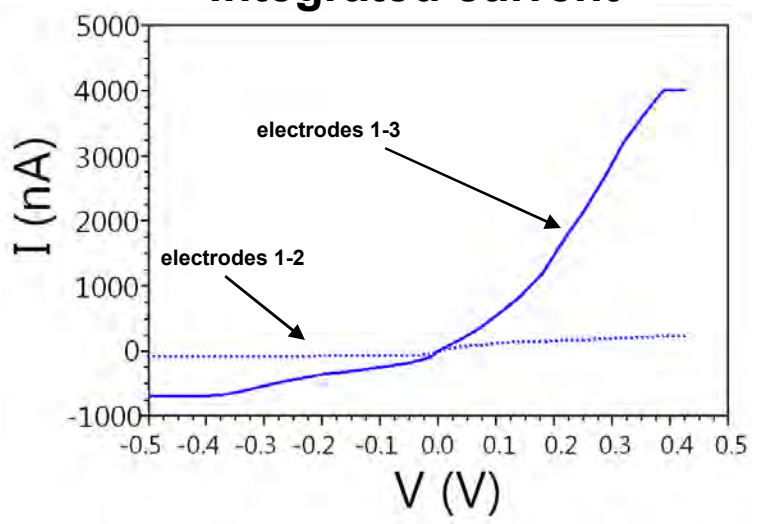
OR gate



Transmission spectrum



Integrated current



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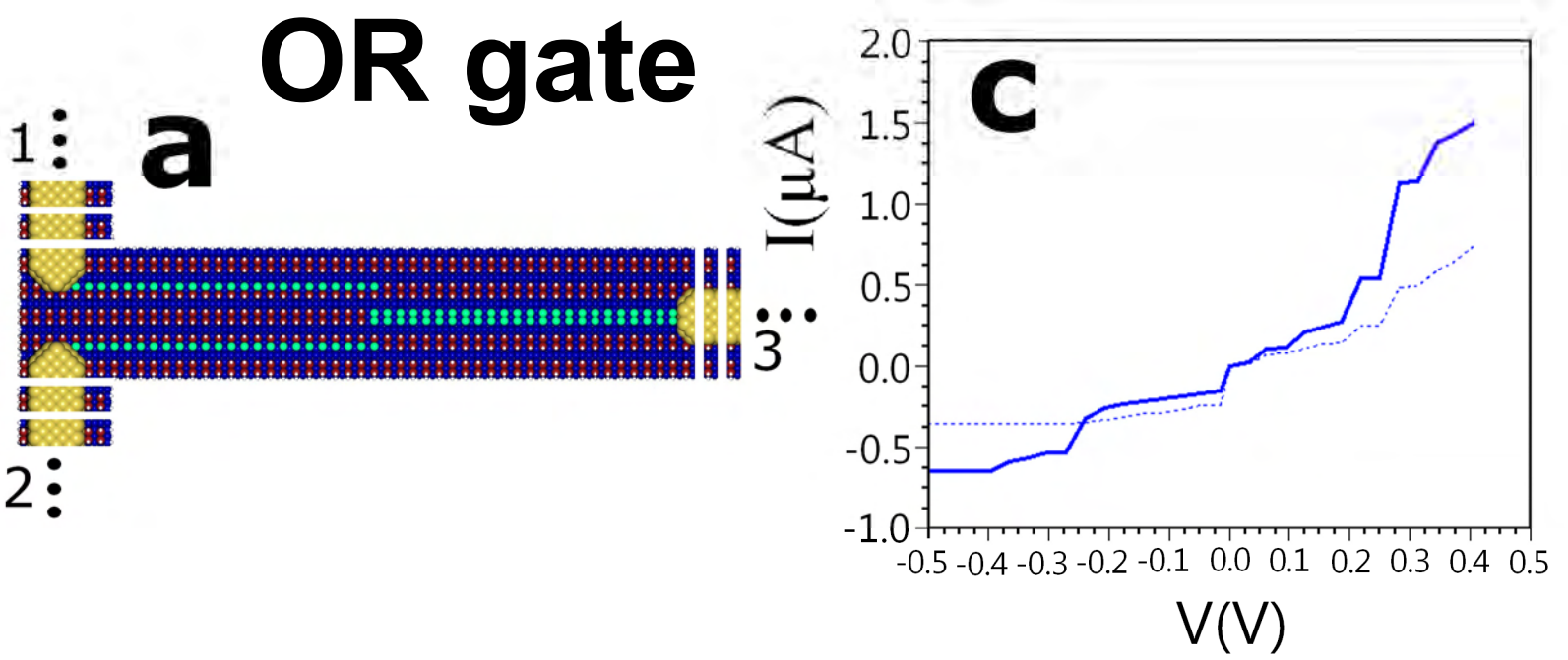
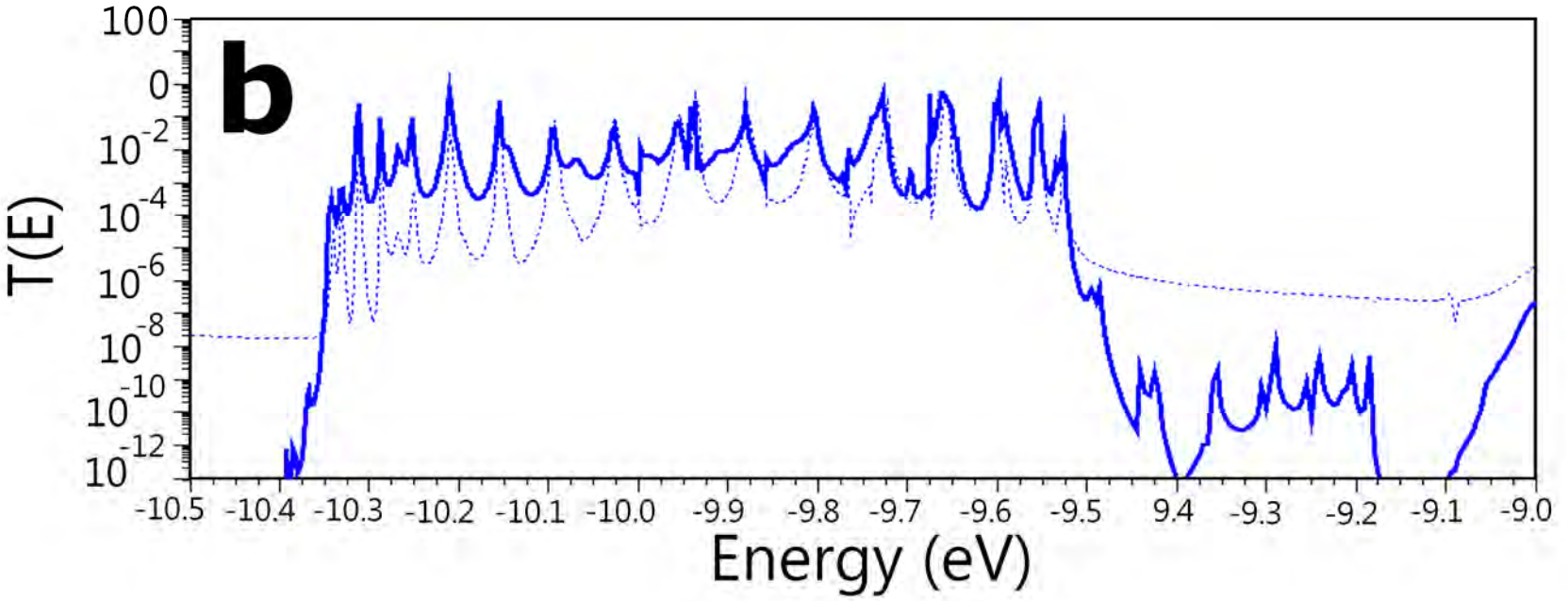
OR gate





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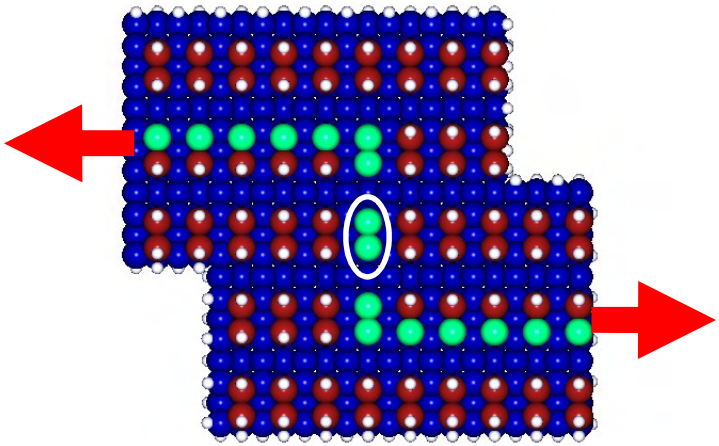
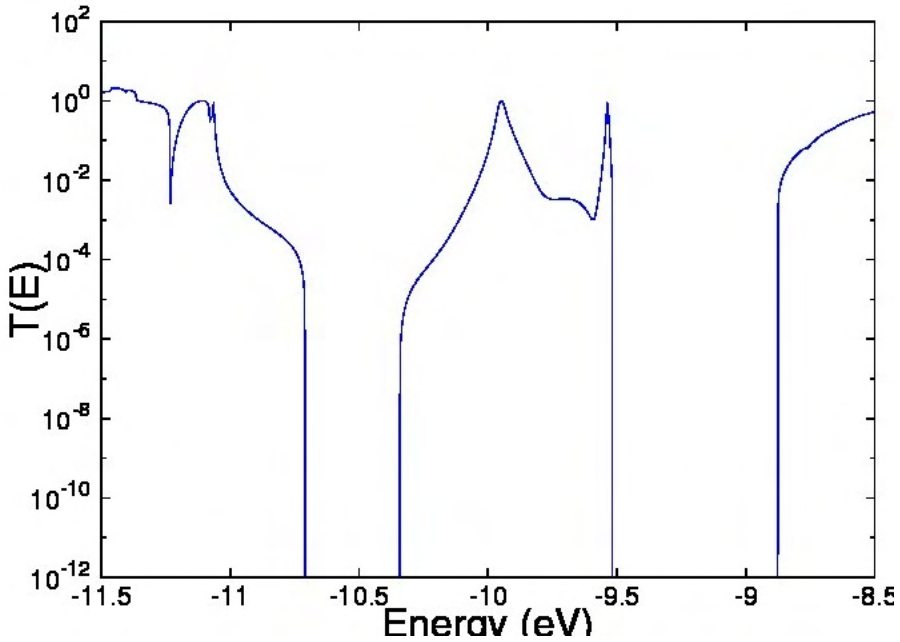
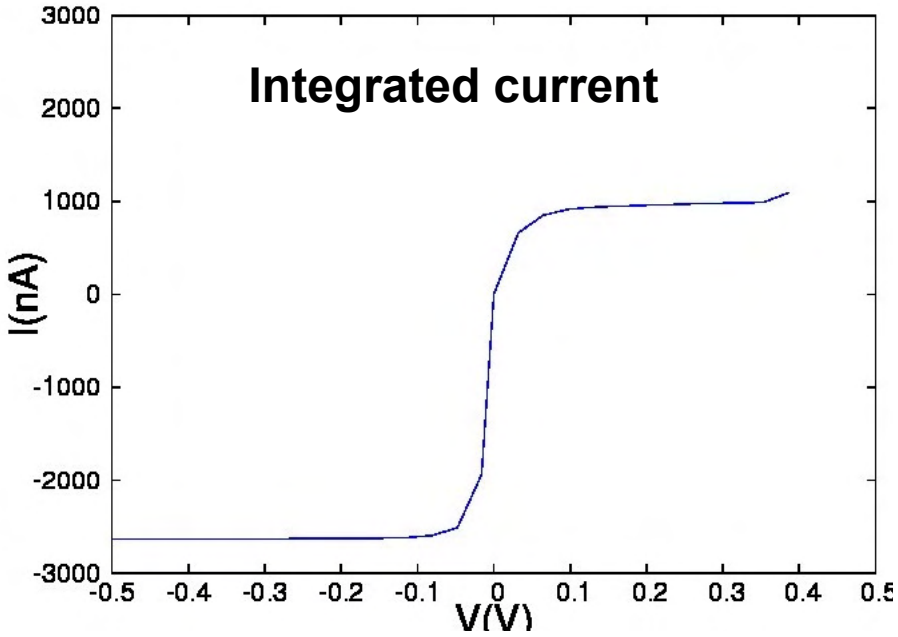
Switch 0 → 1 INVERTER







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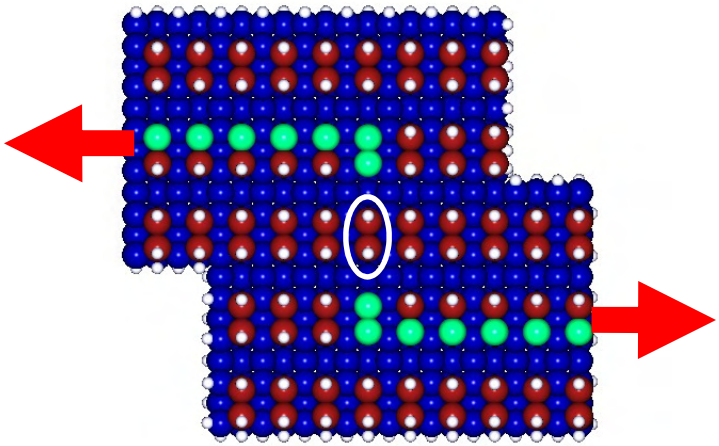

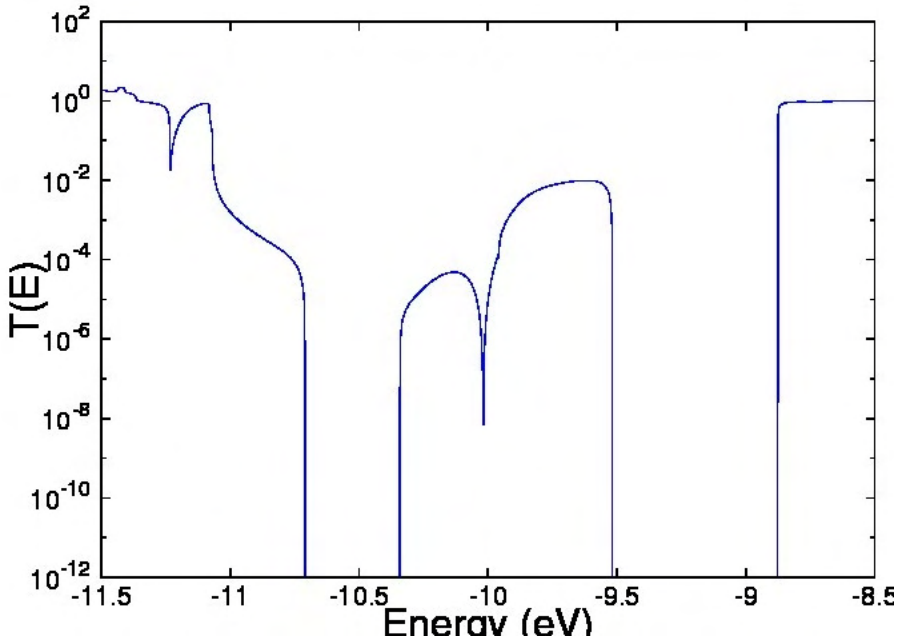

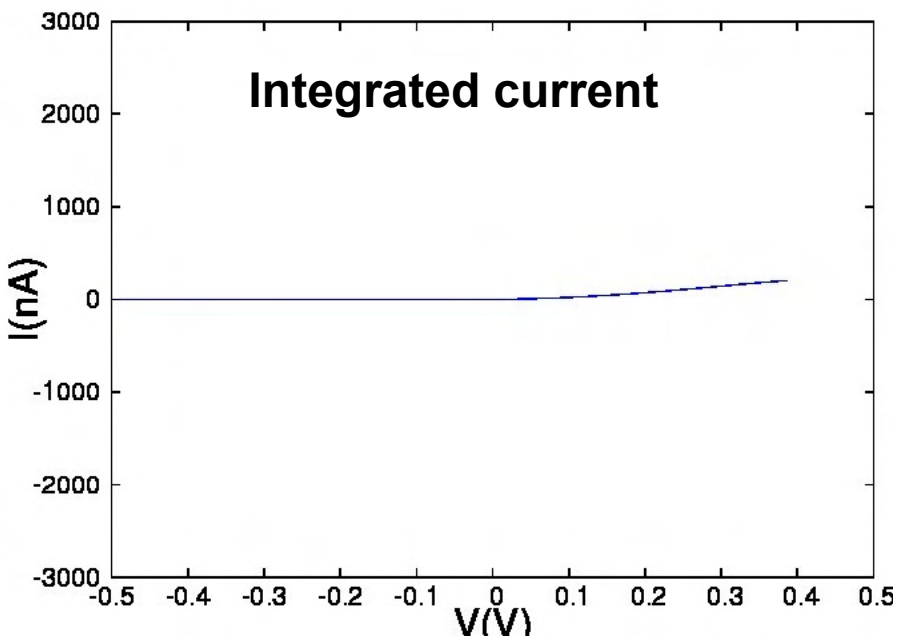

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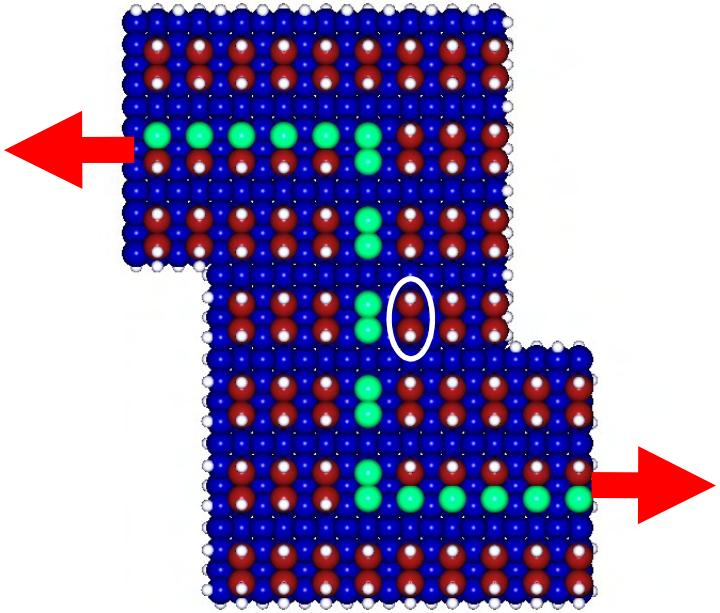

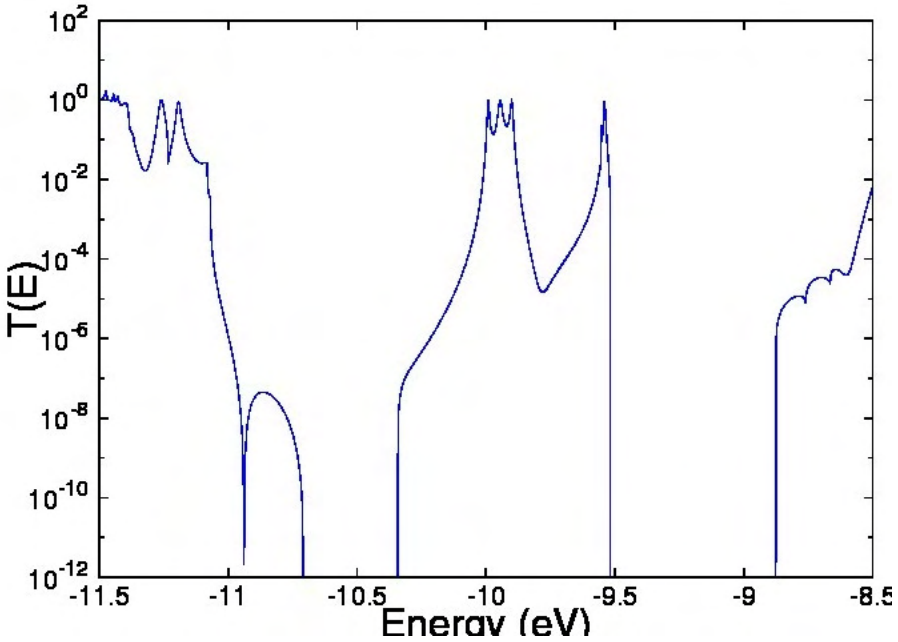

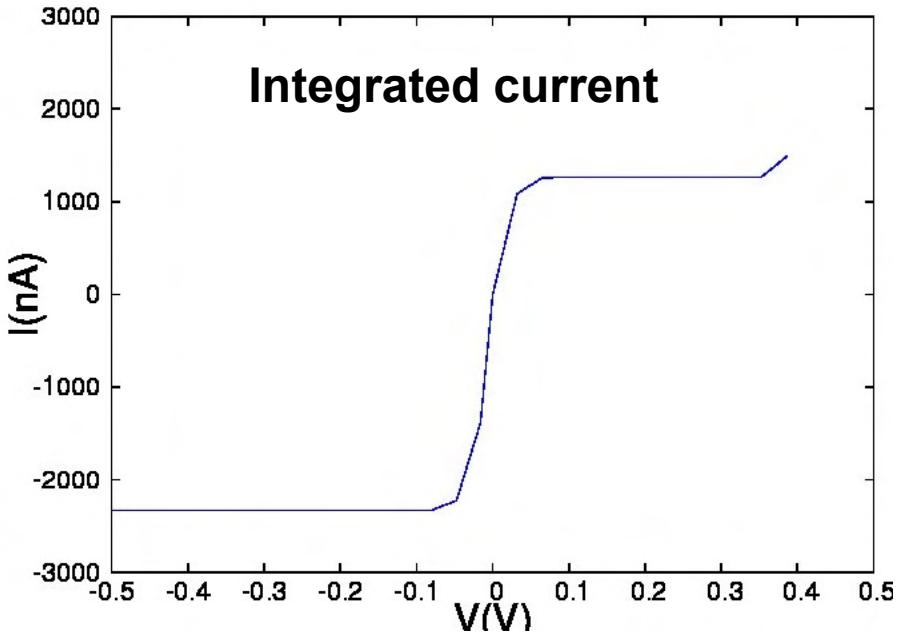

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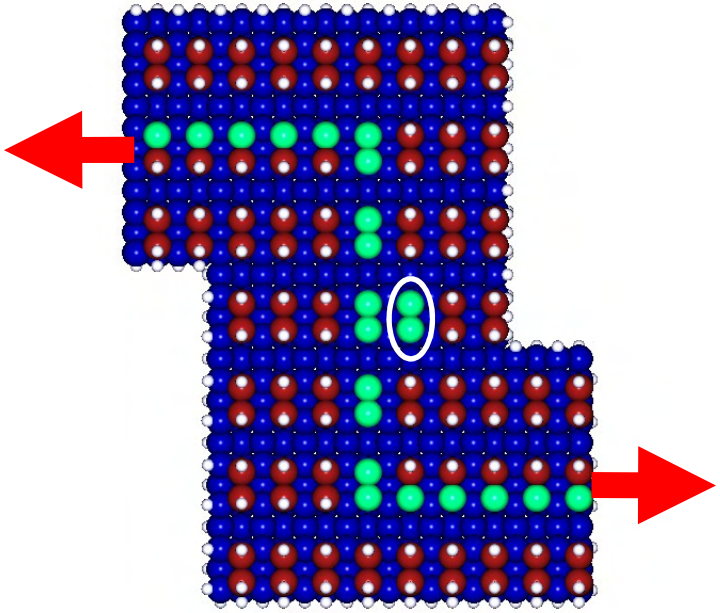

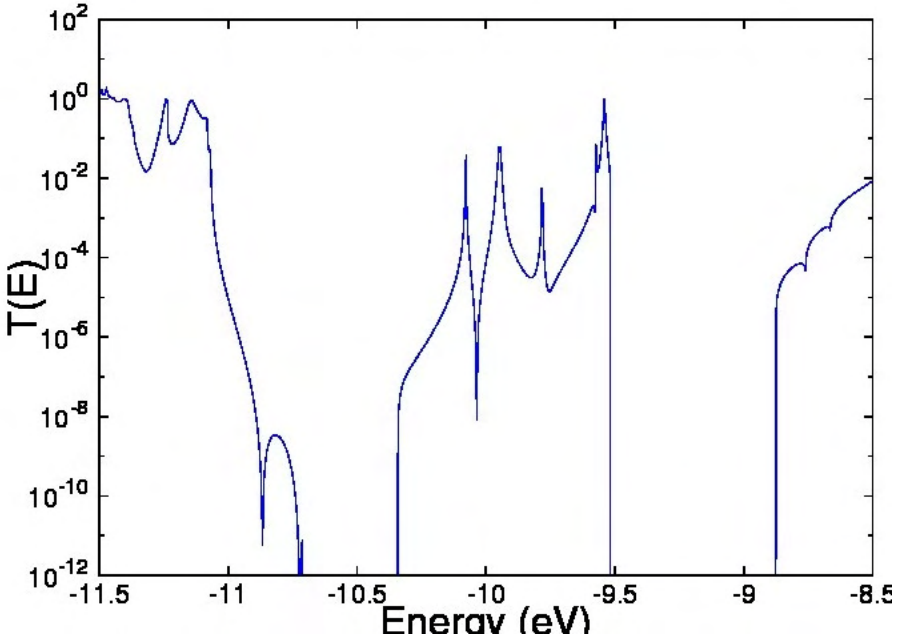

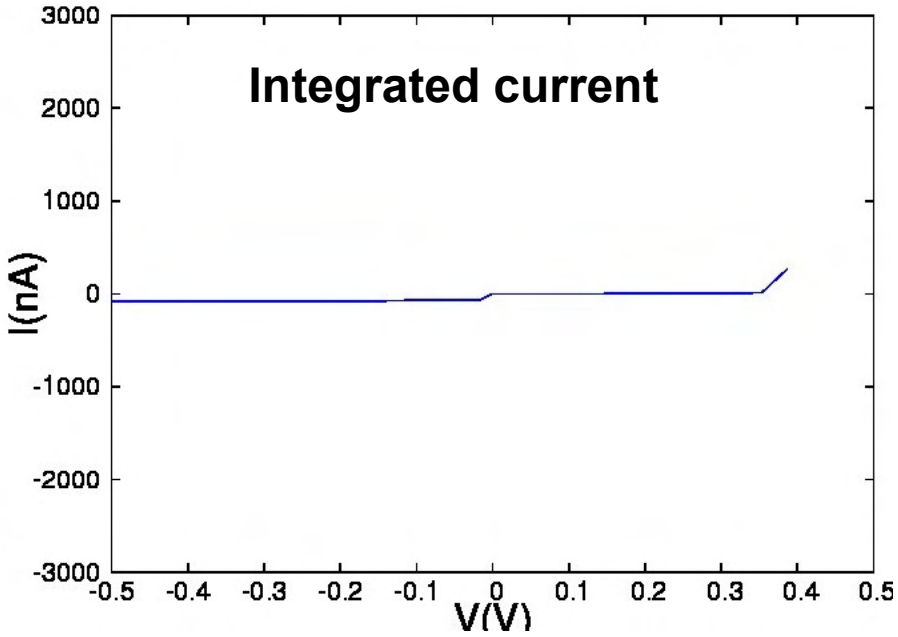

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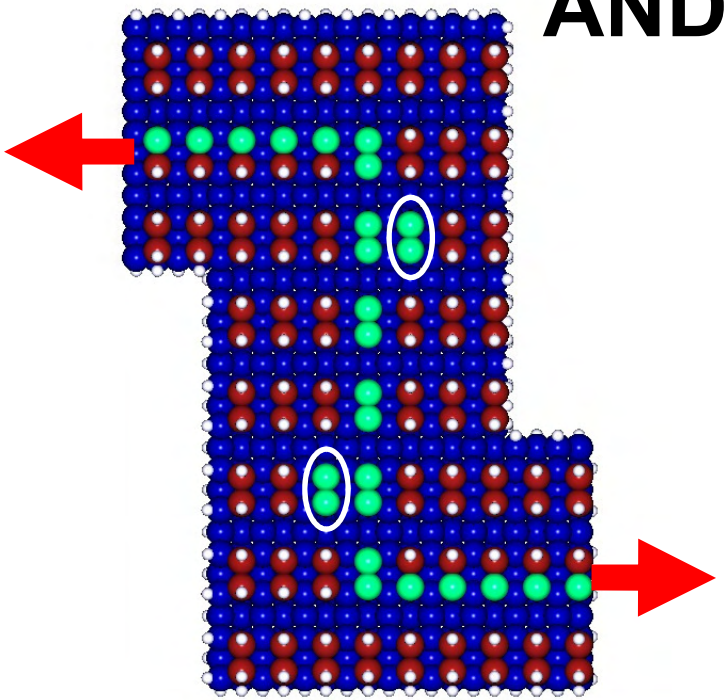

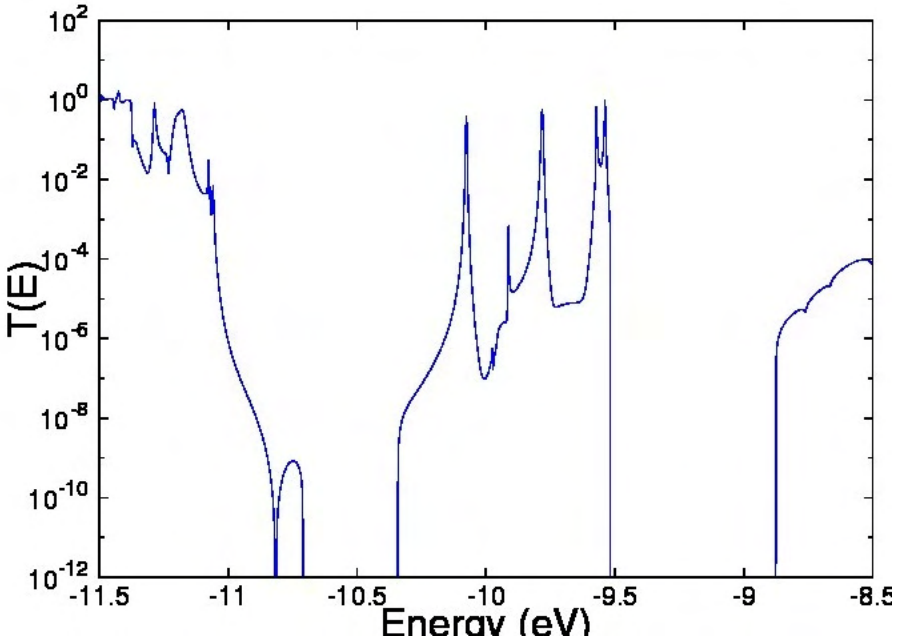

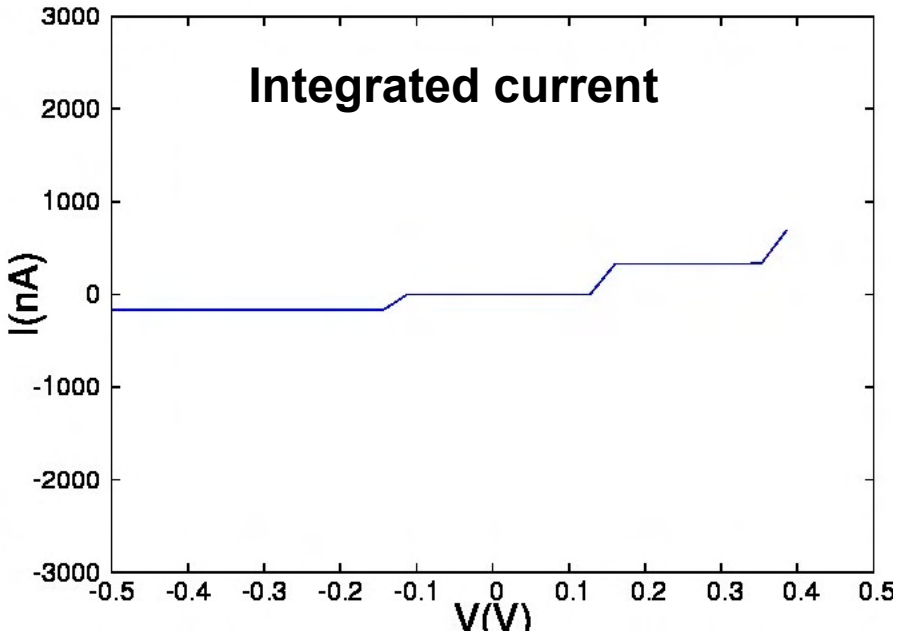

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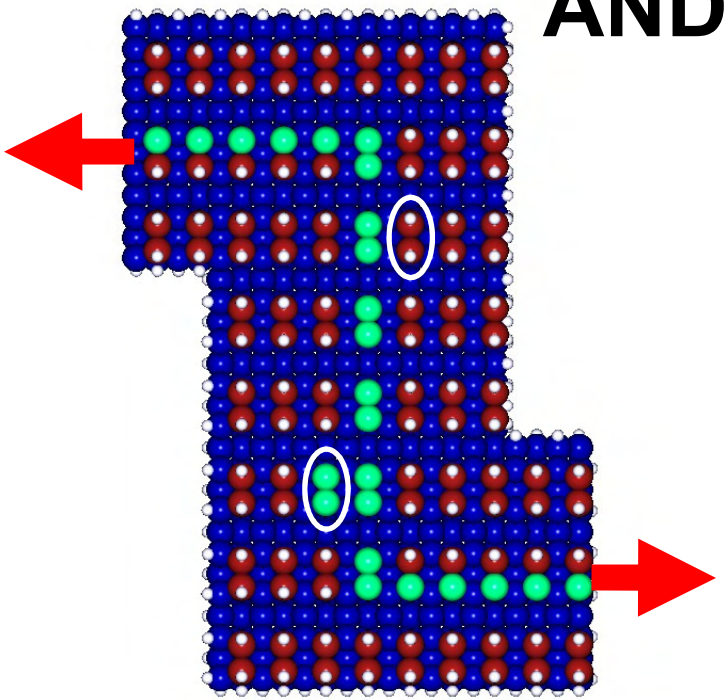

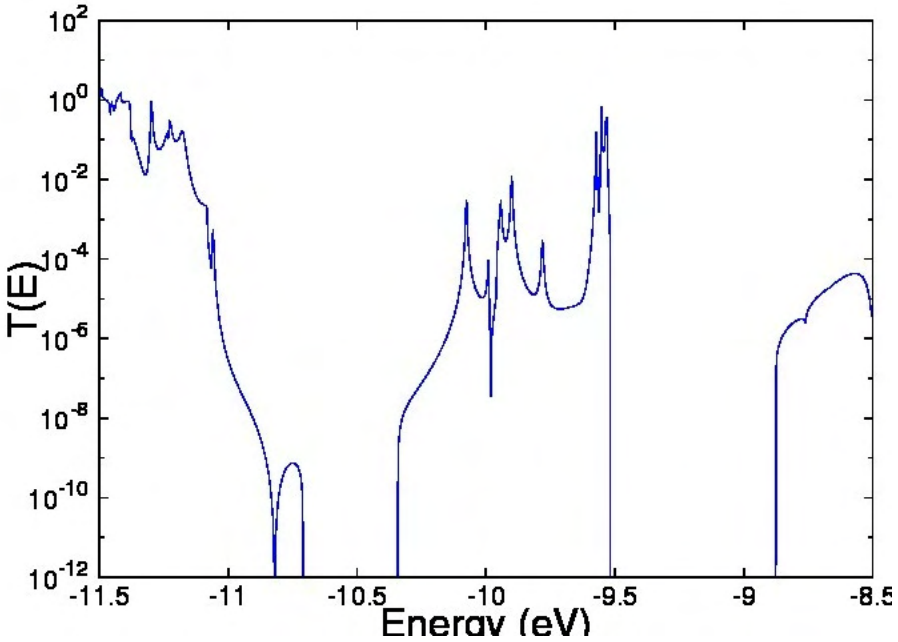

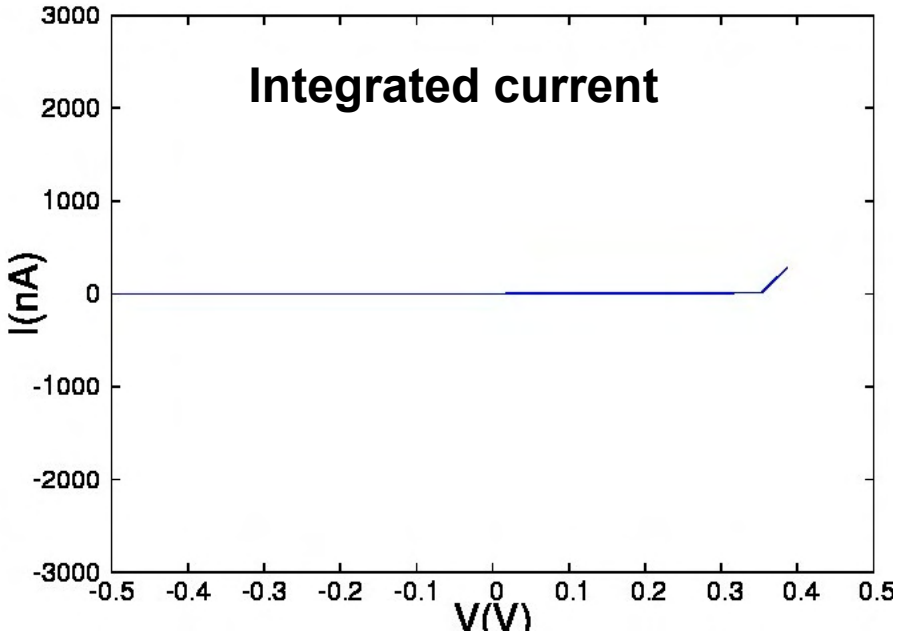

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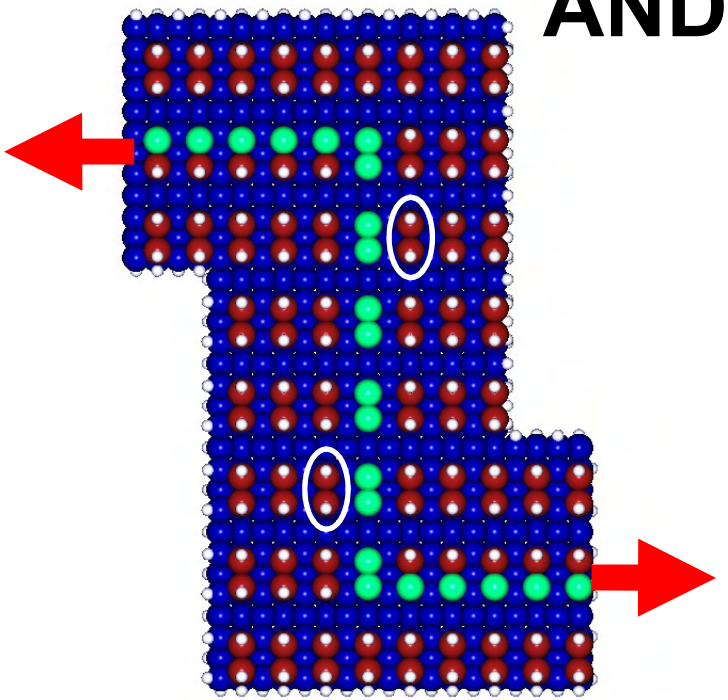

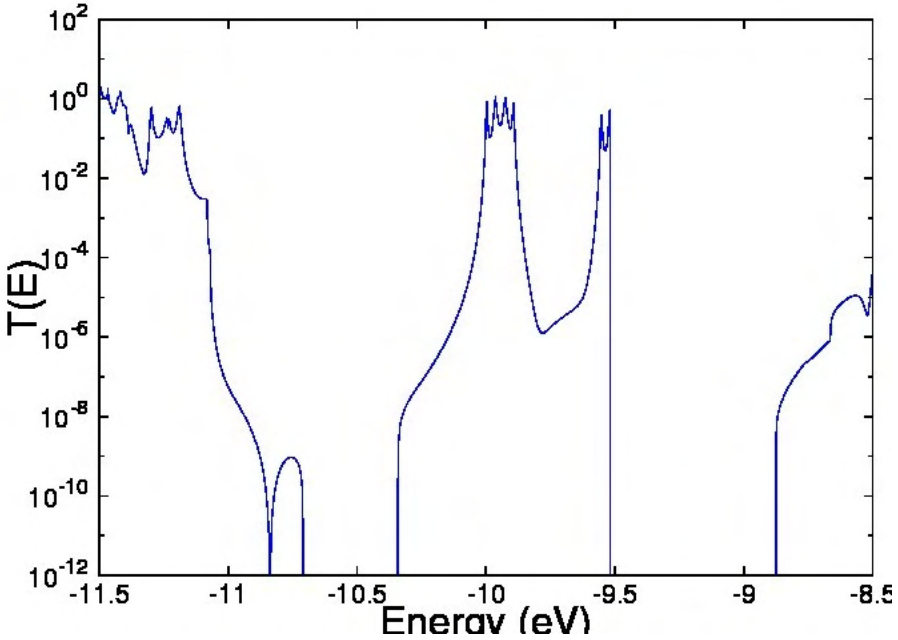

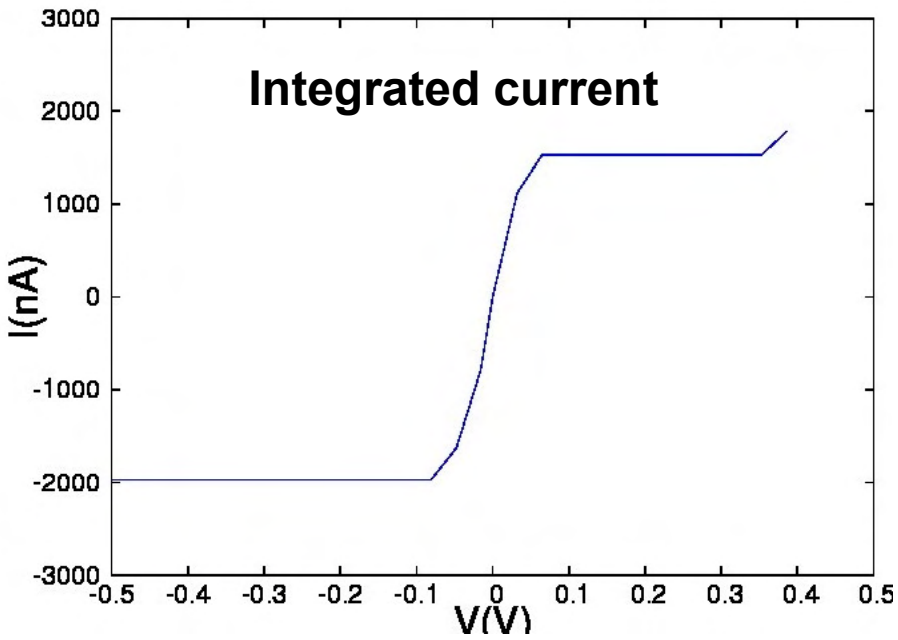

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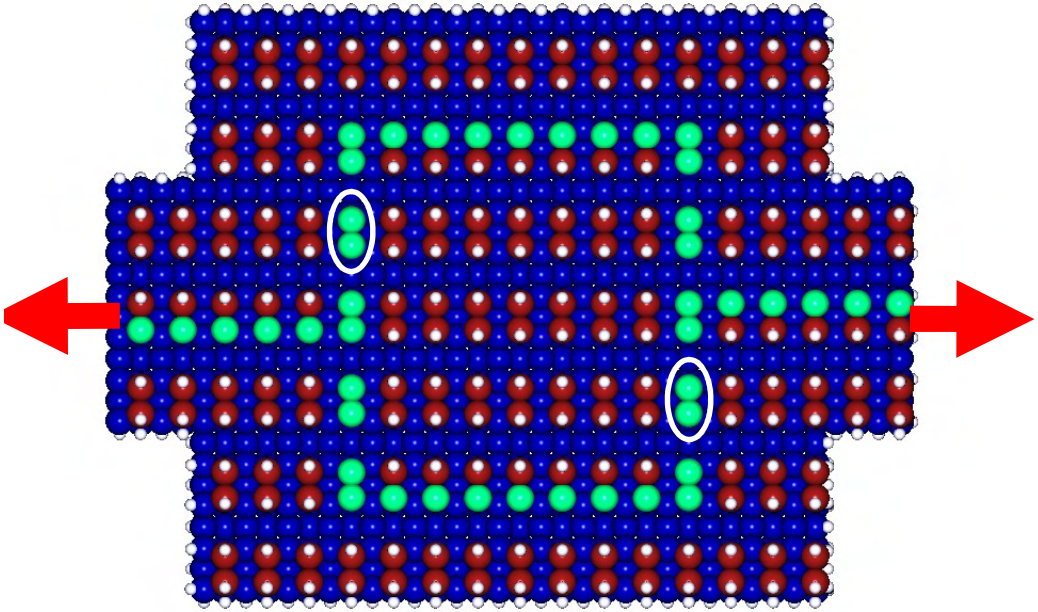

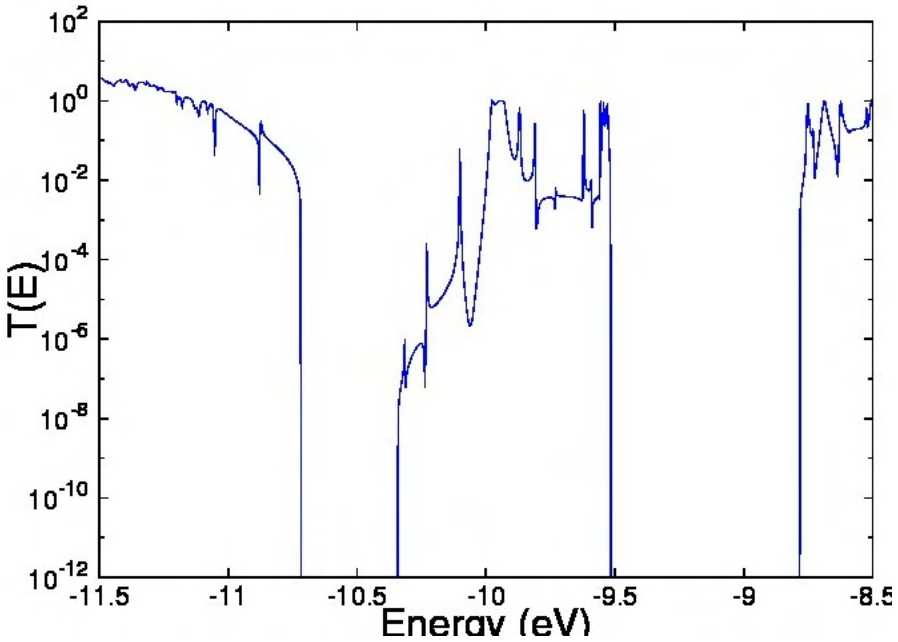

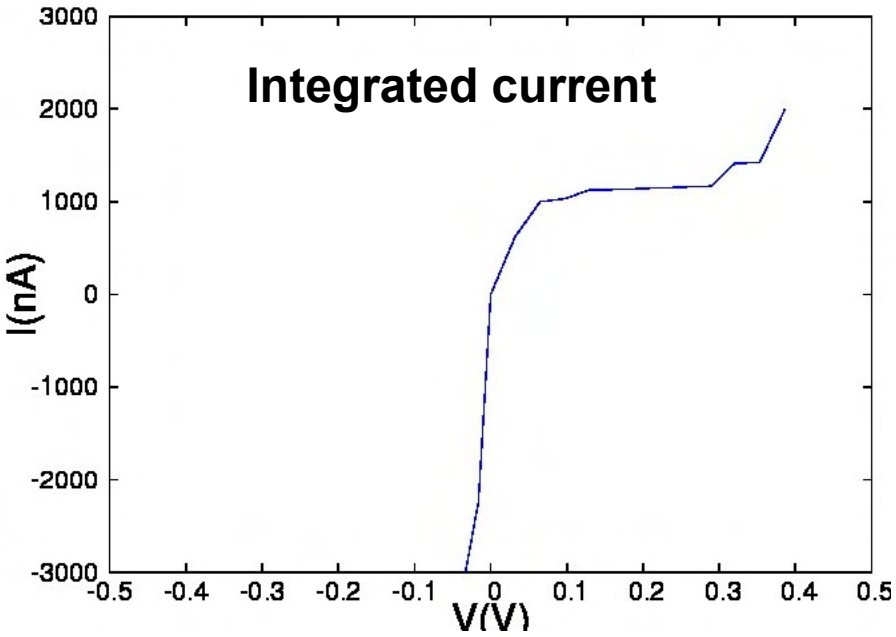

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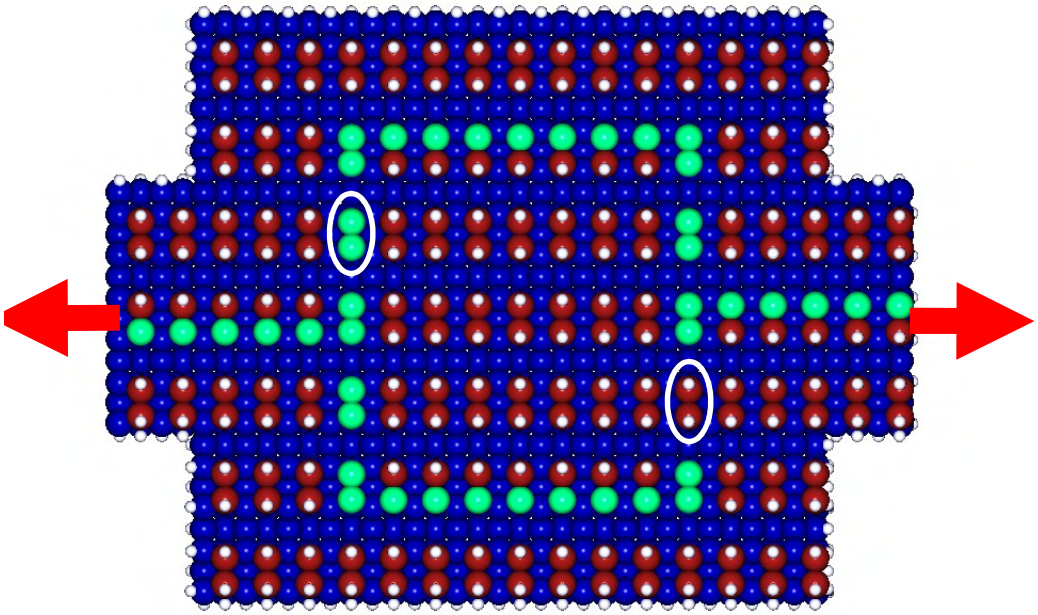

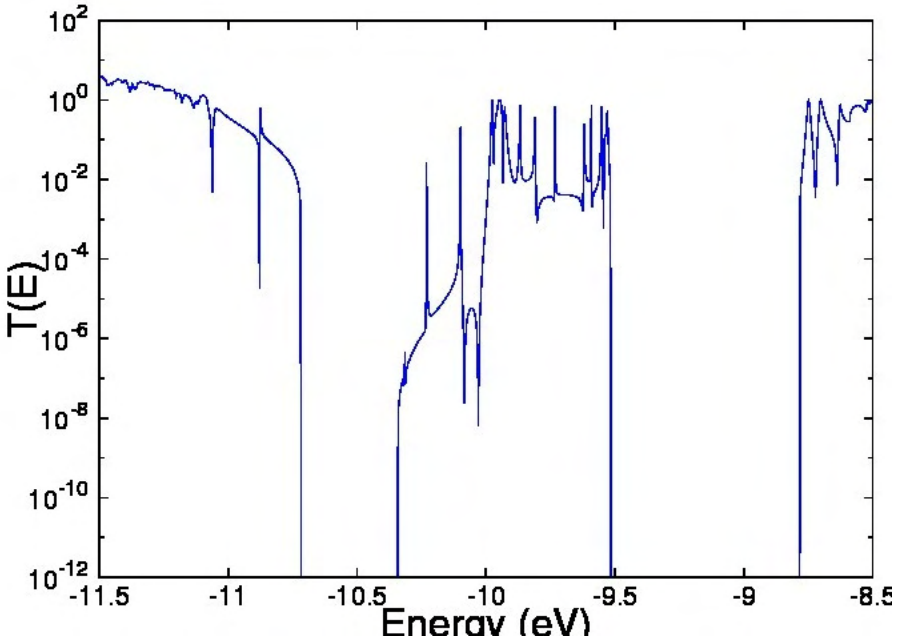

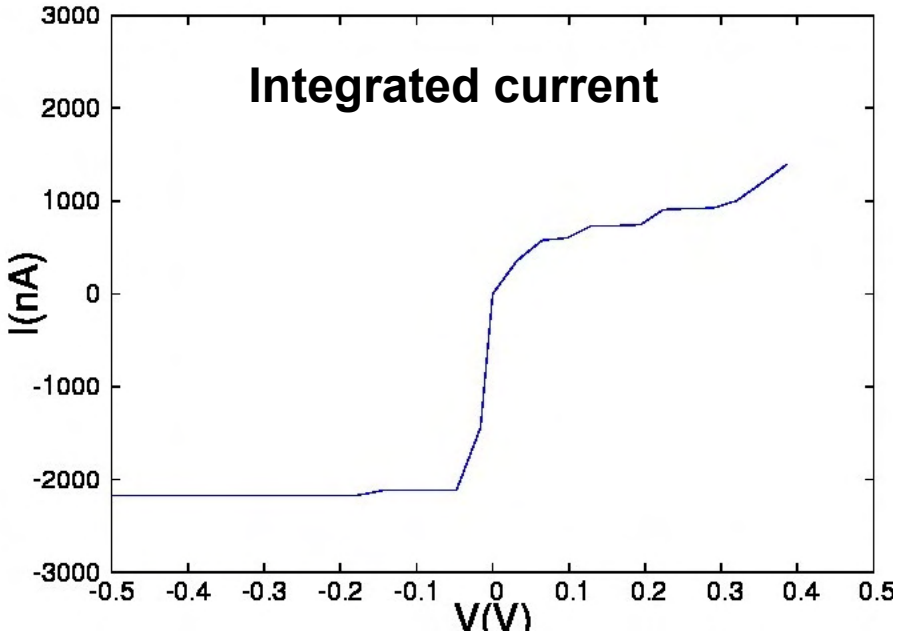

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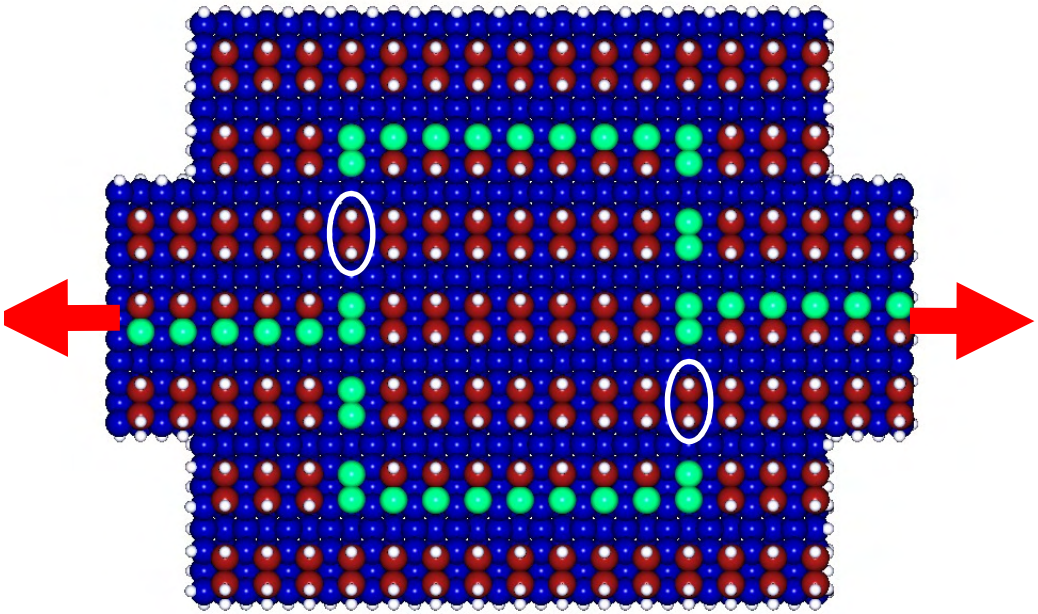
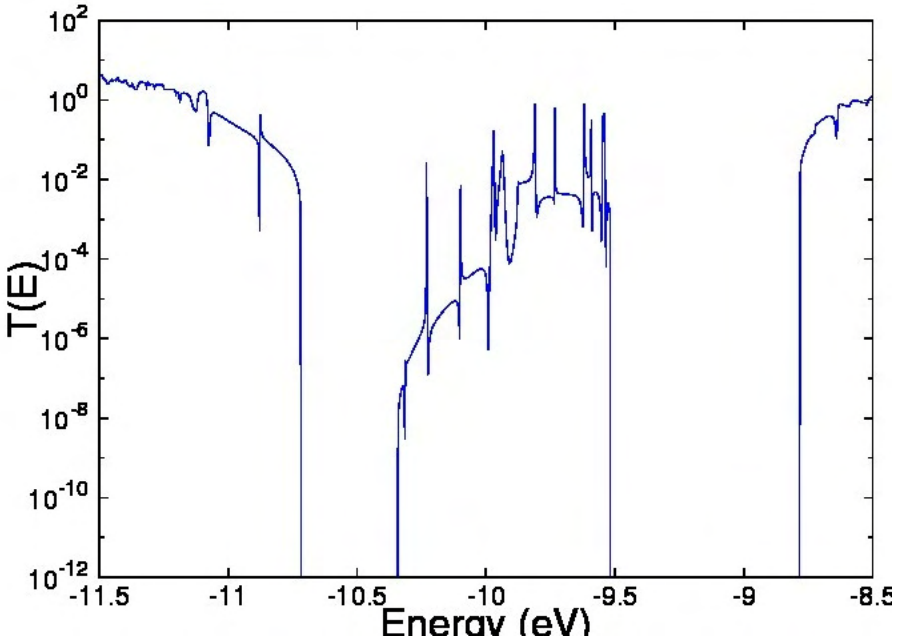
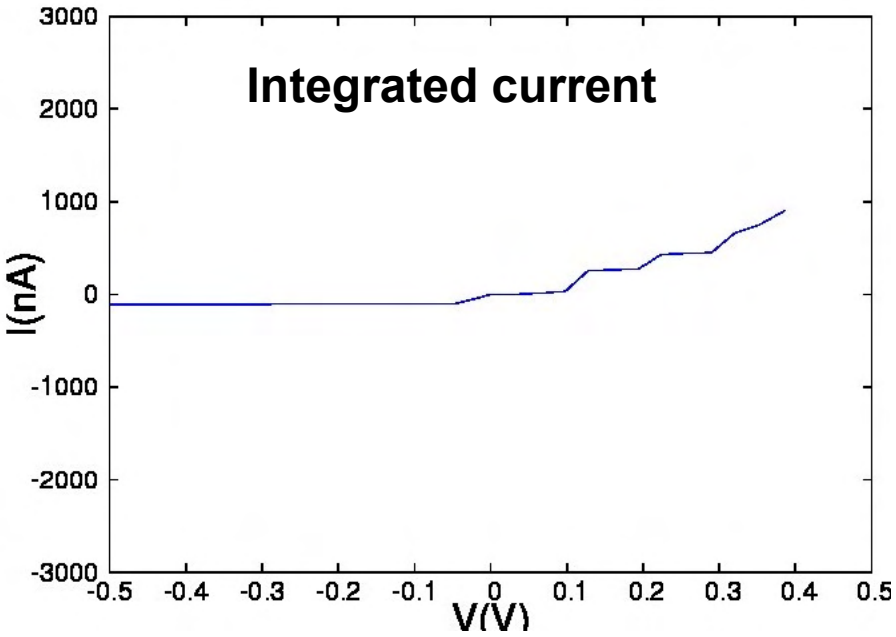
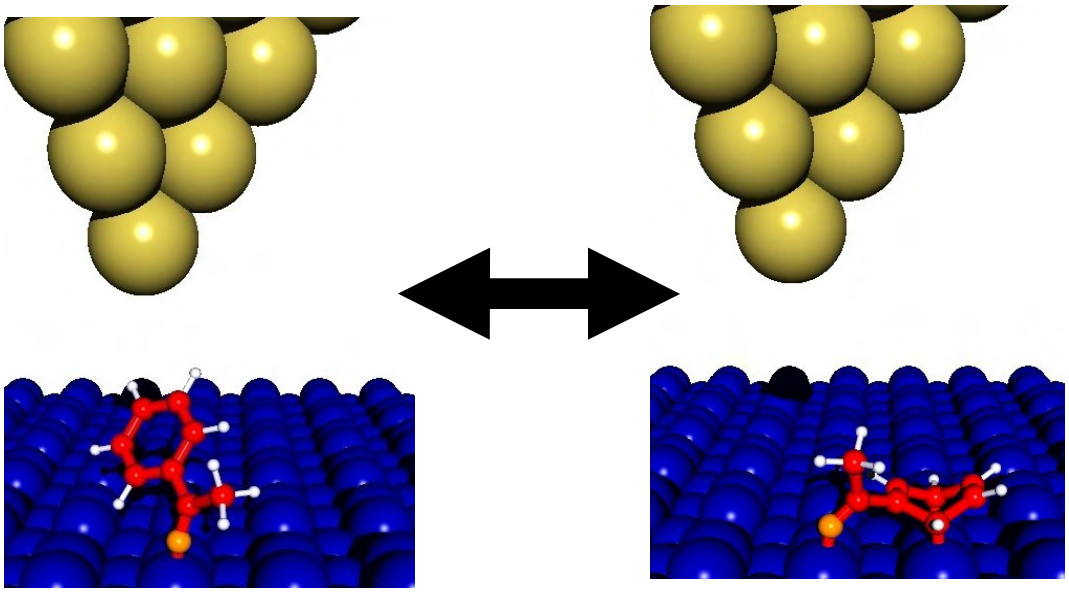






-Theoretical optimization of surface circuits on passivated semiconductors

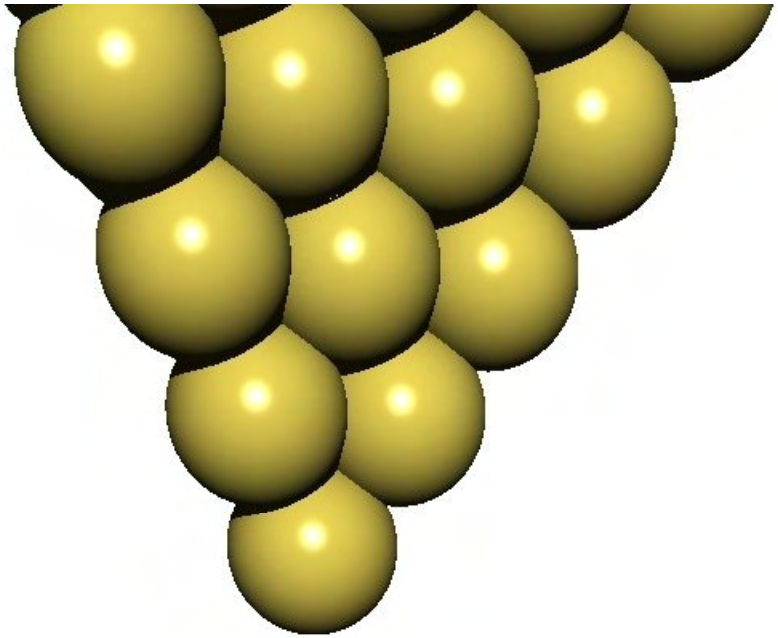
Switch

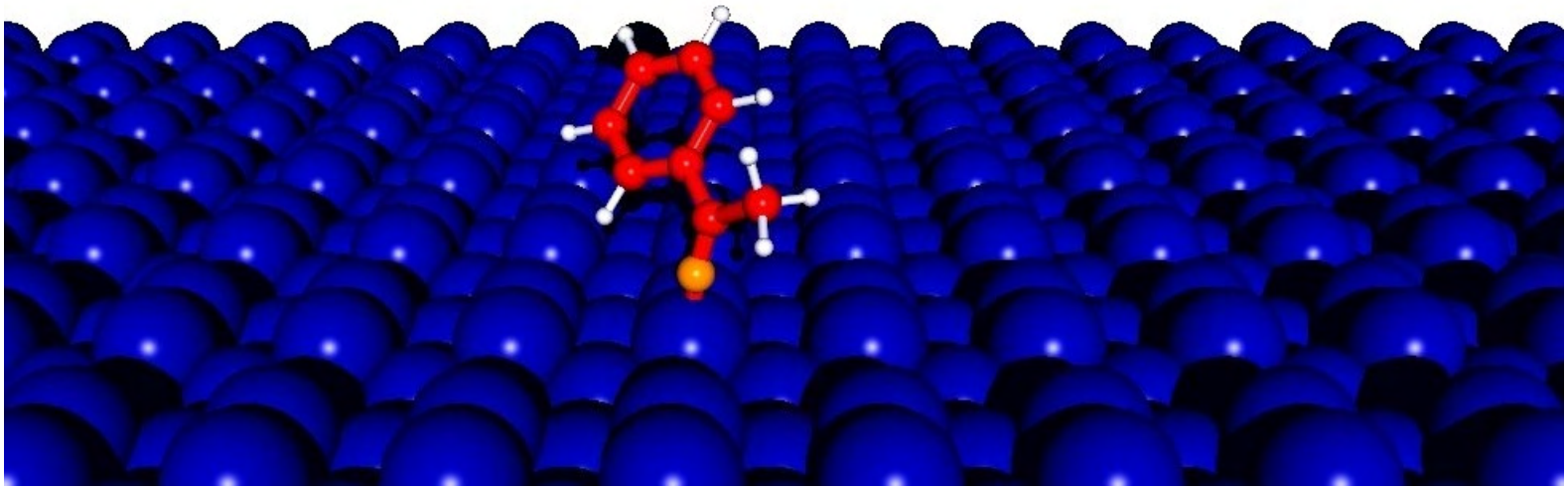


optimized structures with ASED+ approach

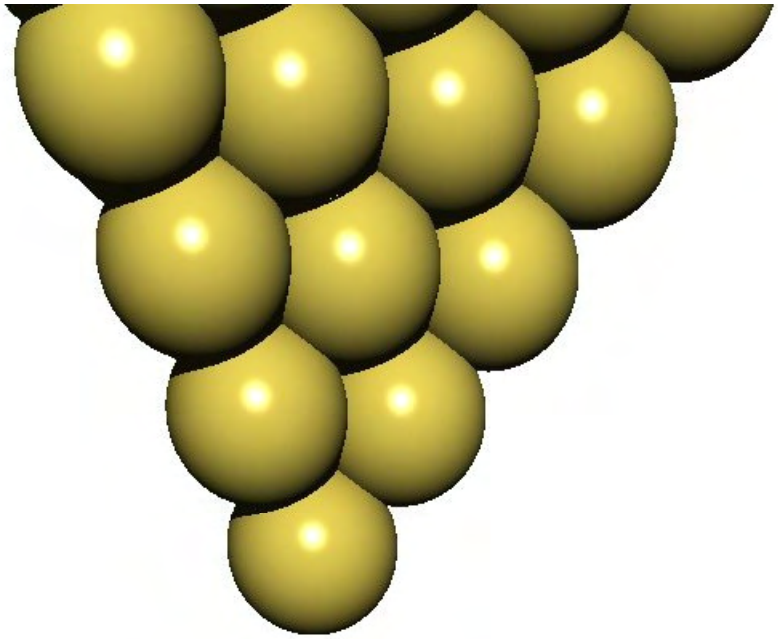
Acetophenone can switch on Si(100) by the inelastic forces of the STM current.

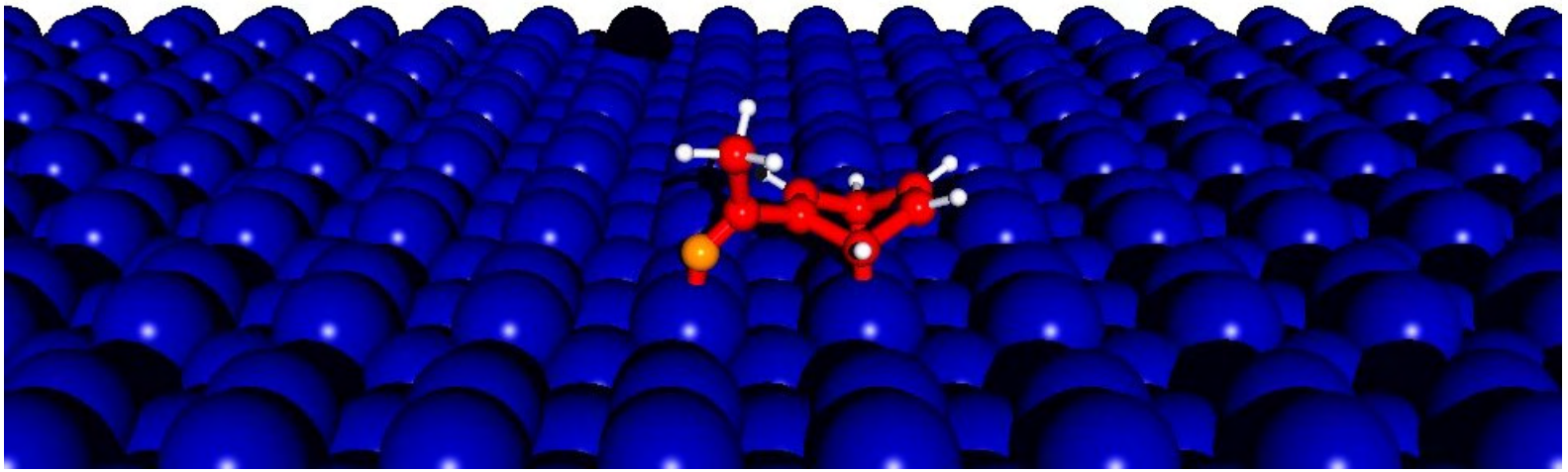
Acetophenone on Si(100)



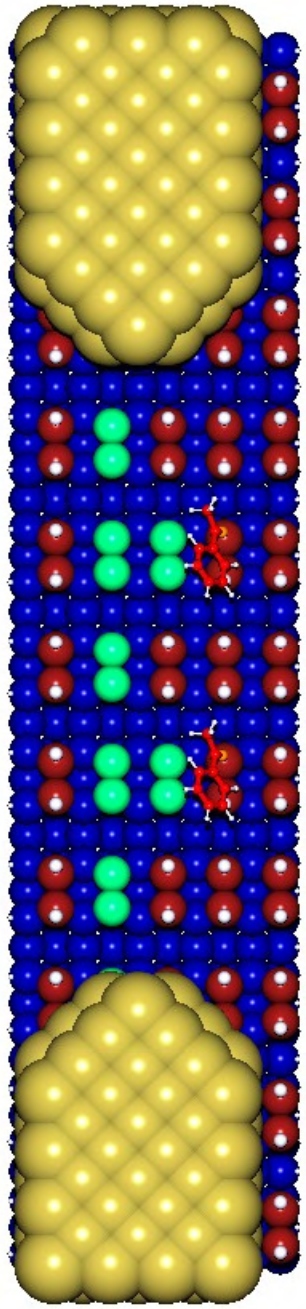


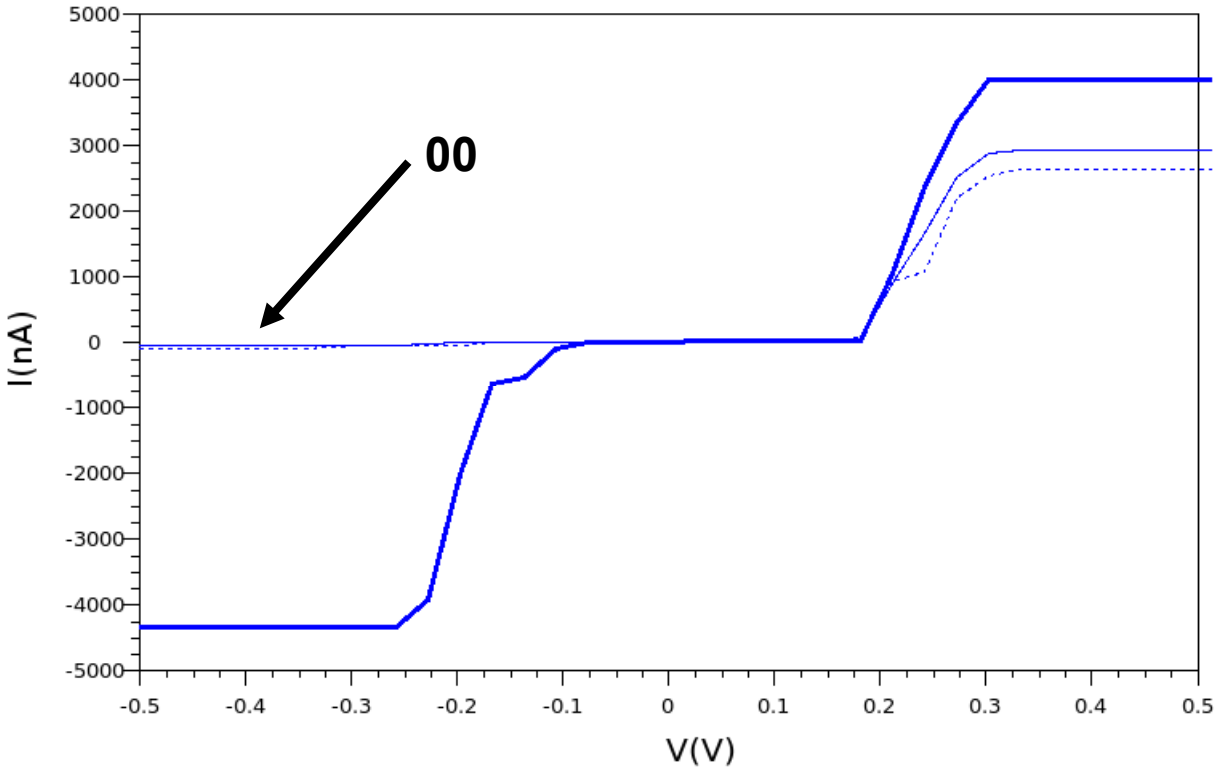
Acetophenone on Si(100)





-Theoretical optimization of surface circuits on passivated semiconductors





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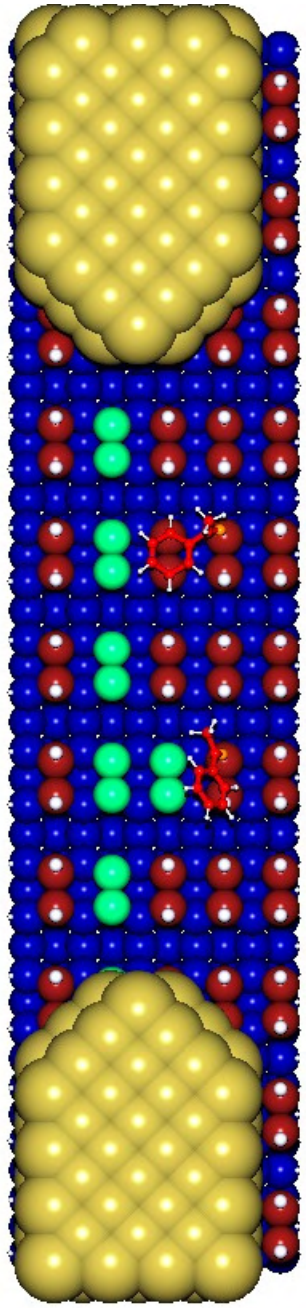
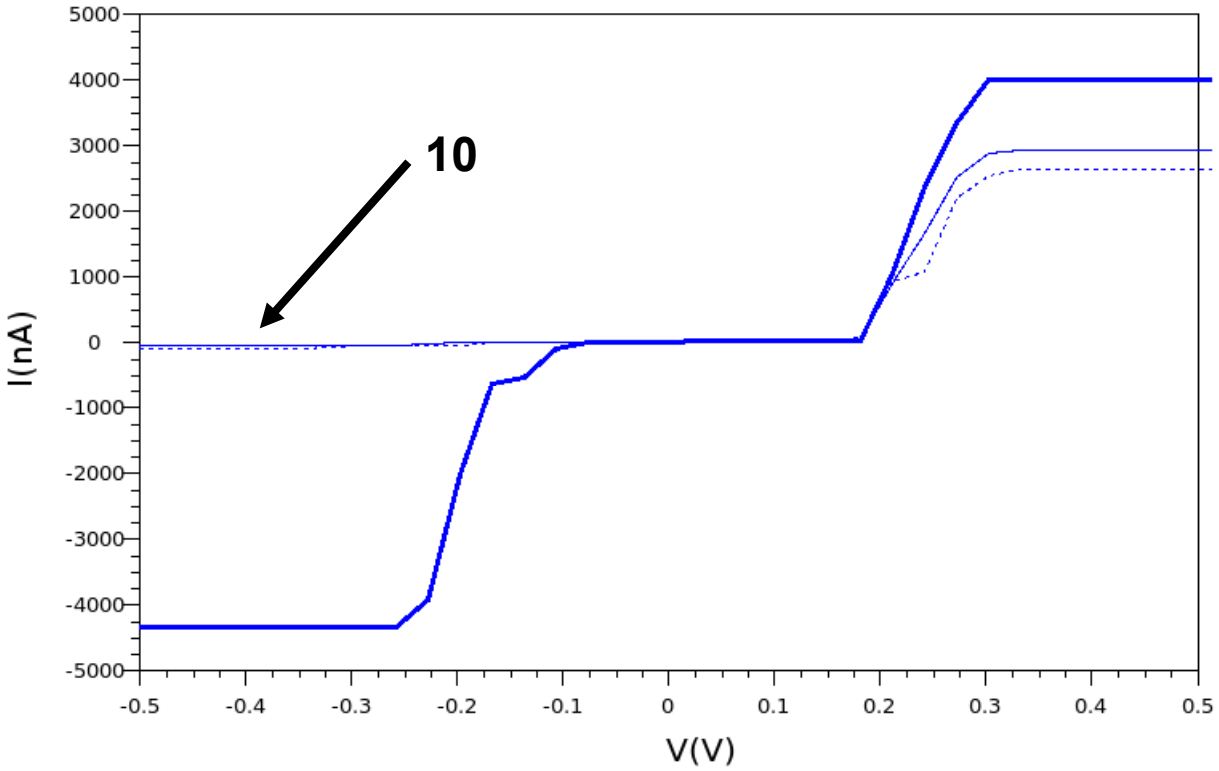
-Theoretical optimization of surface circuits on passivated semiconductors





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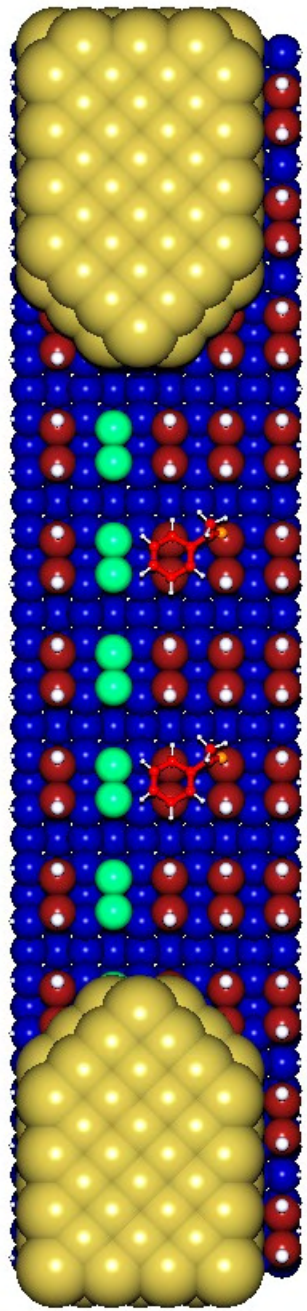
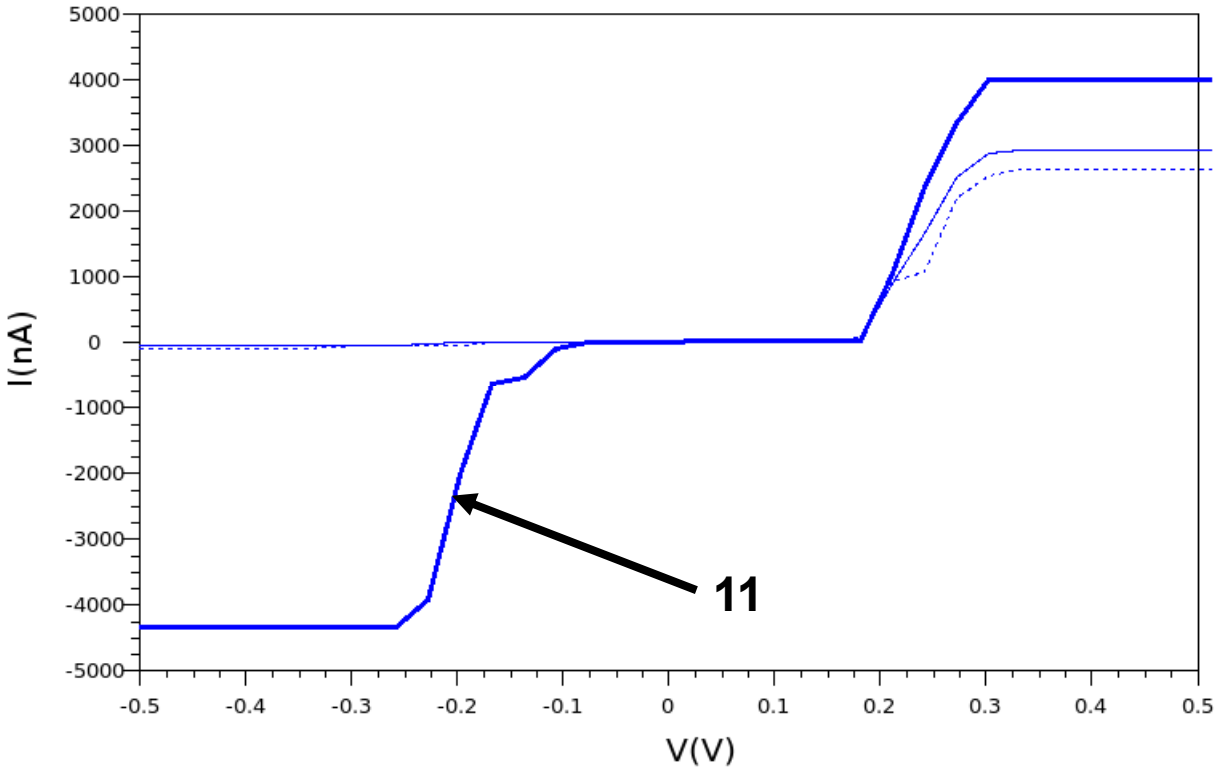
-Theoretical optimization of surface circuits on passivated semiconductors





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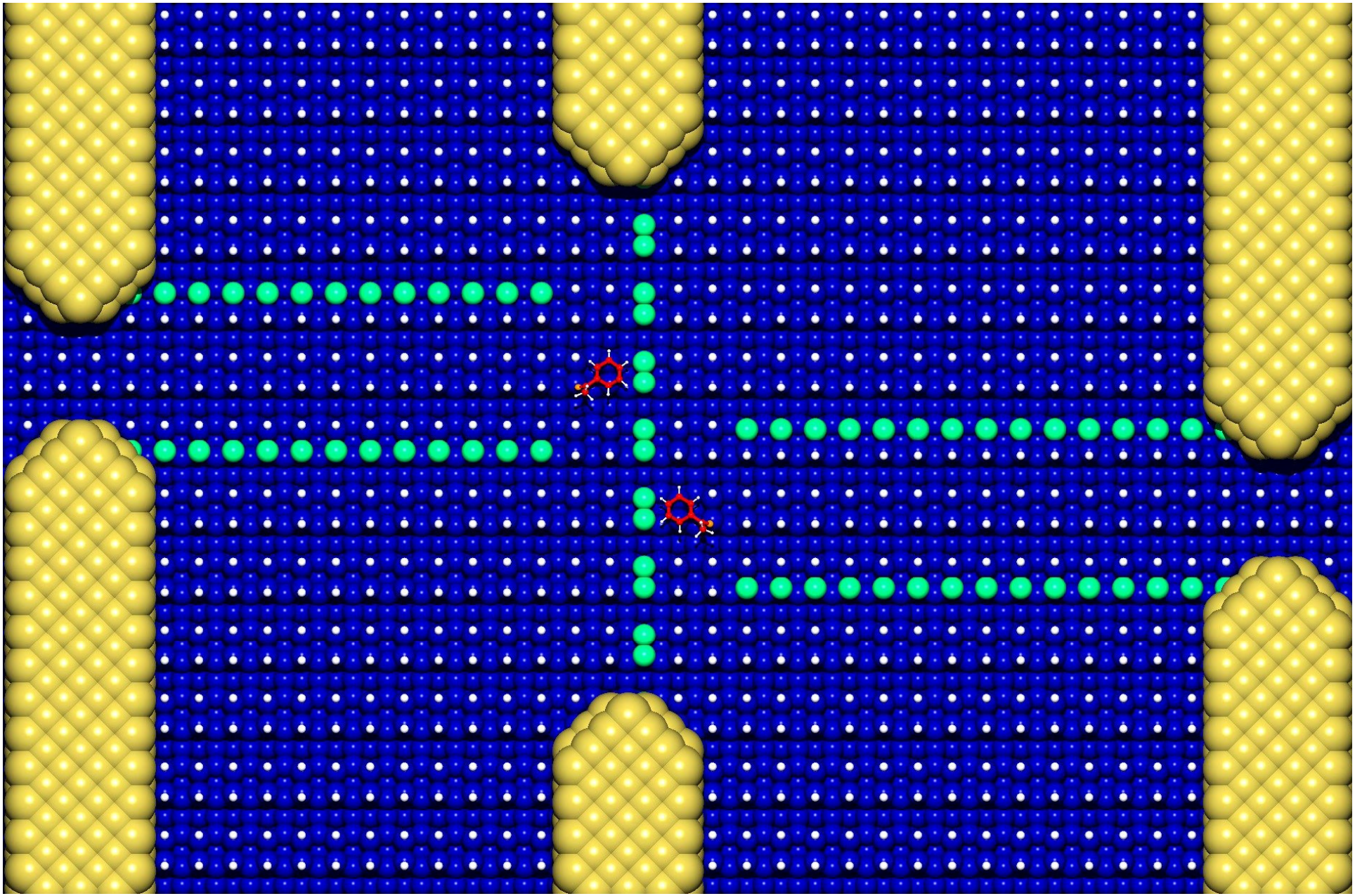
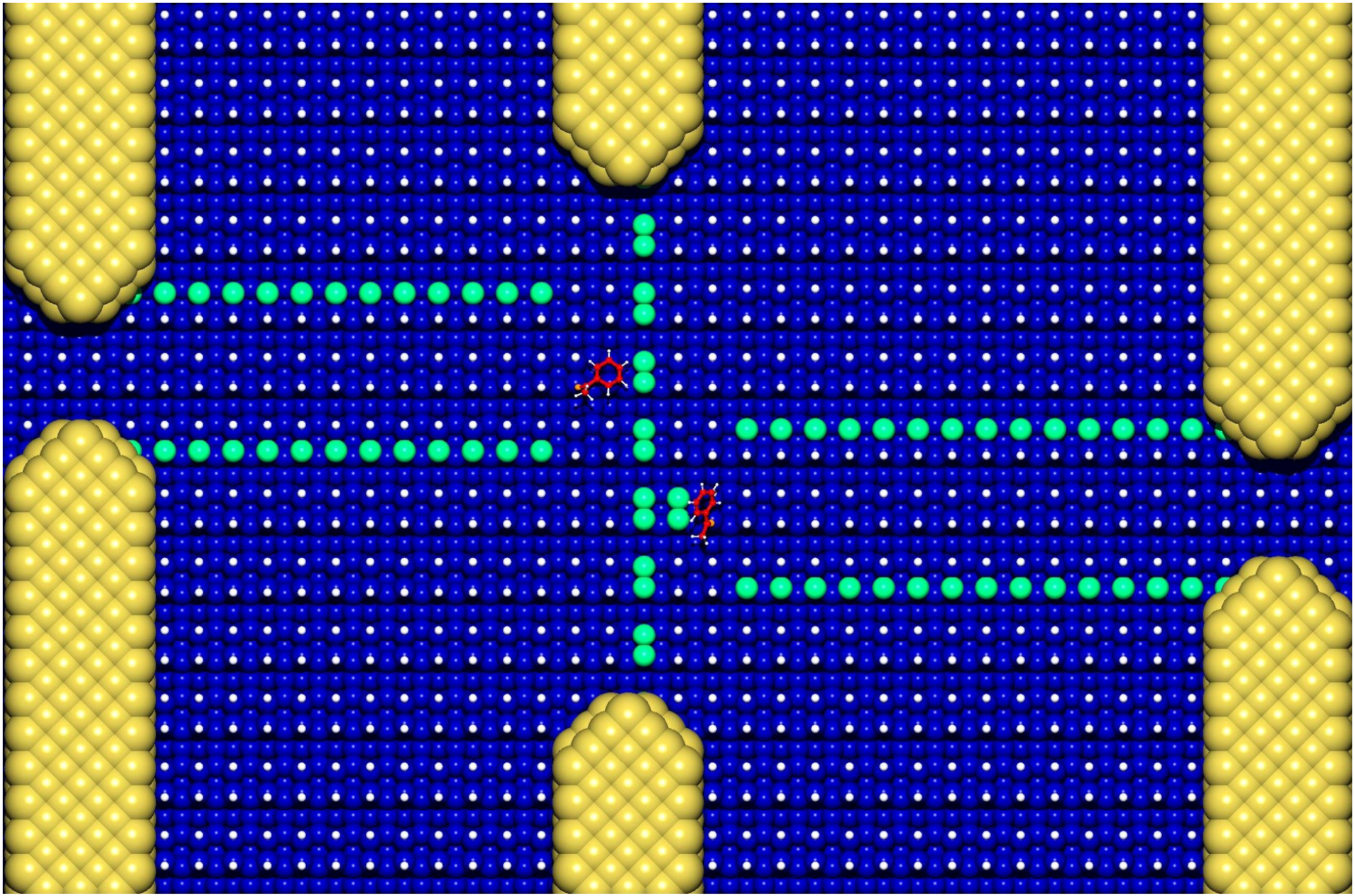
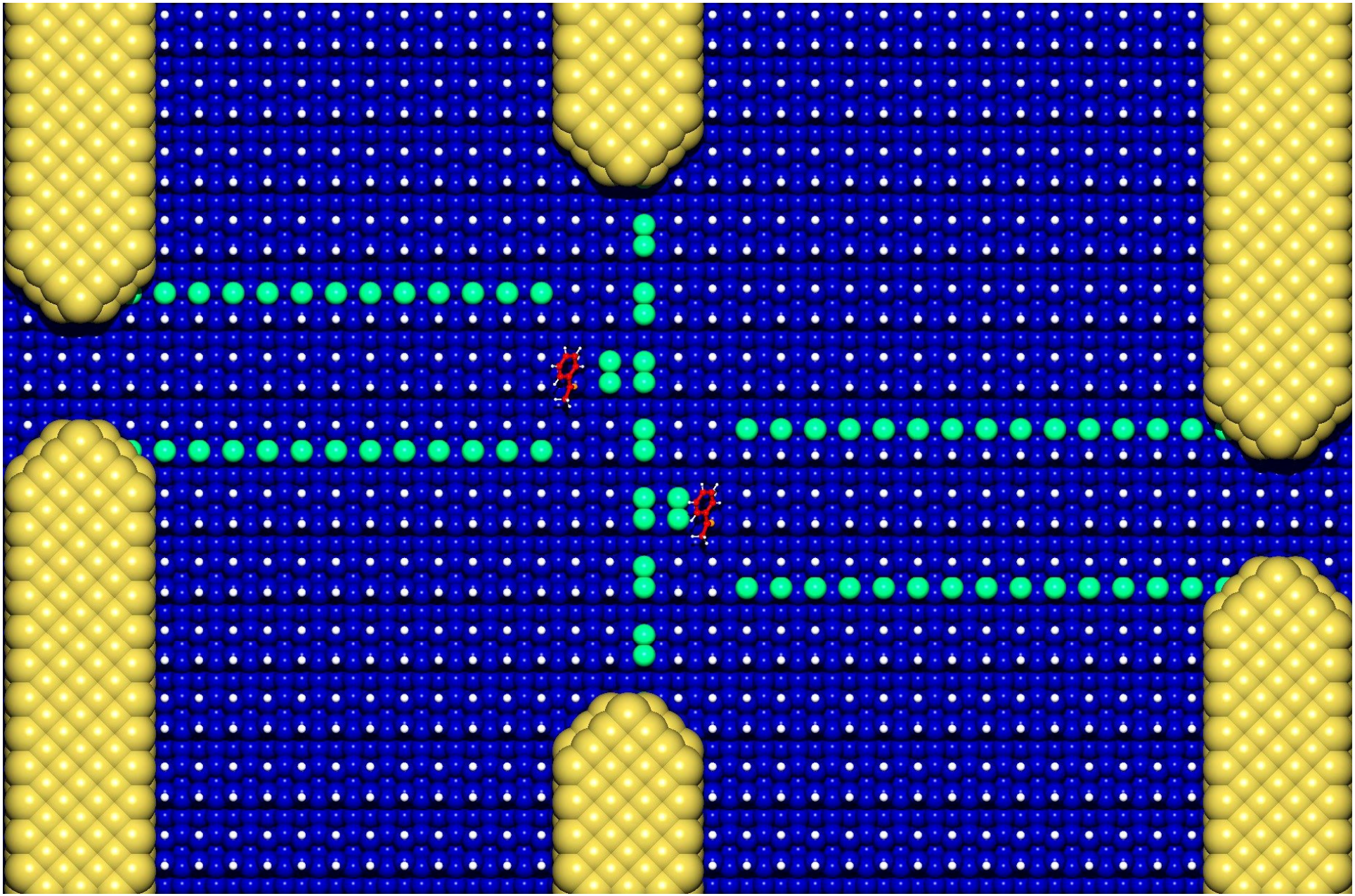
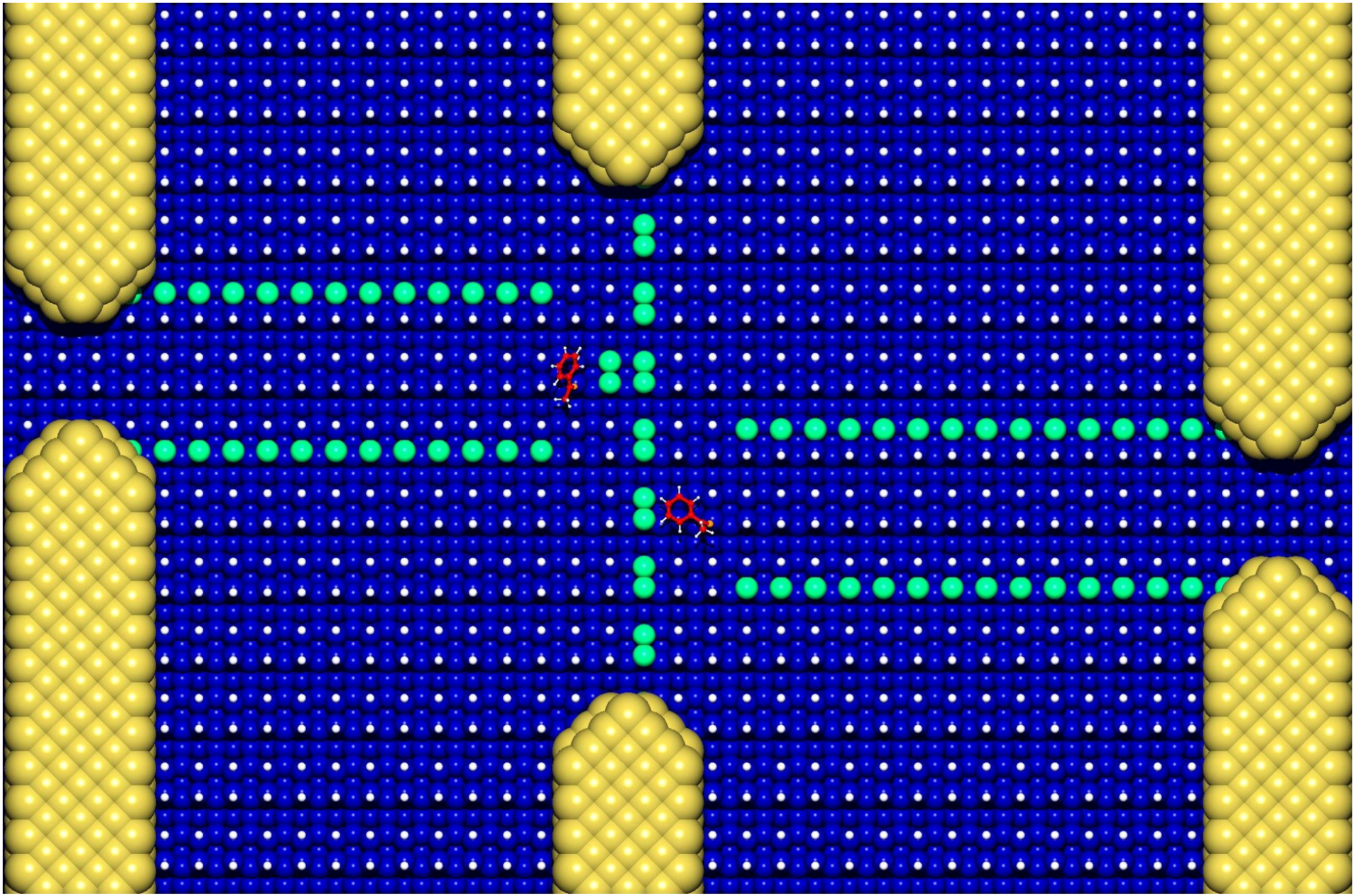
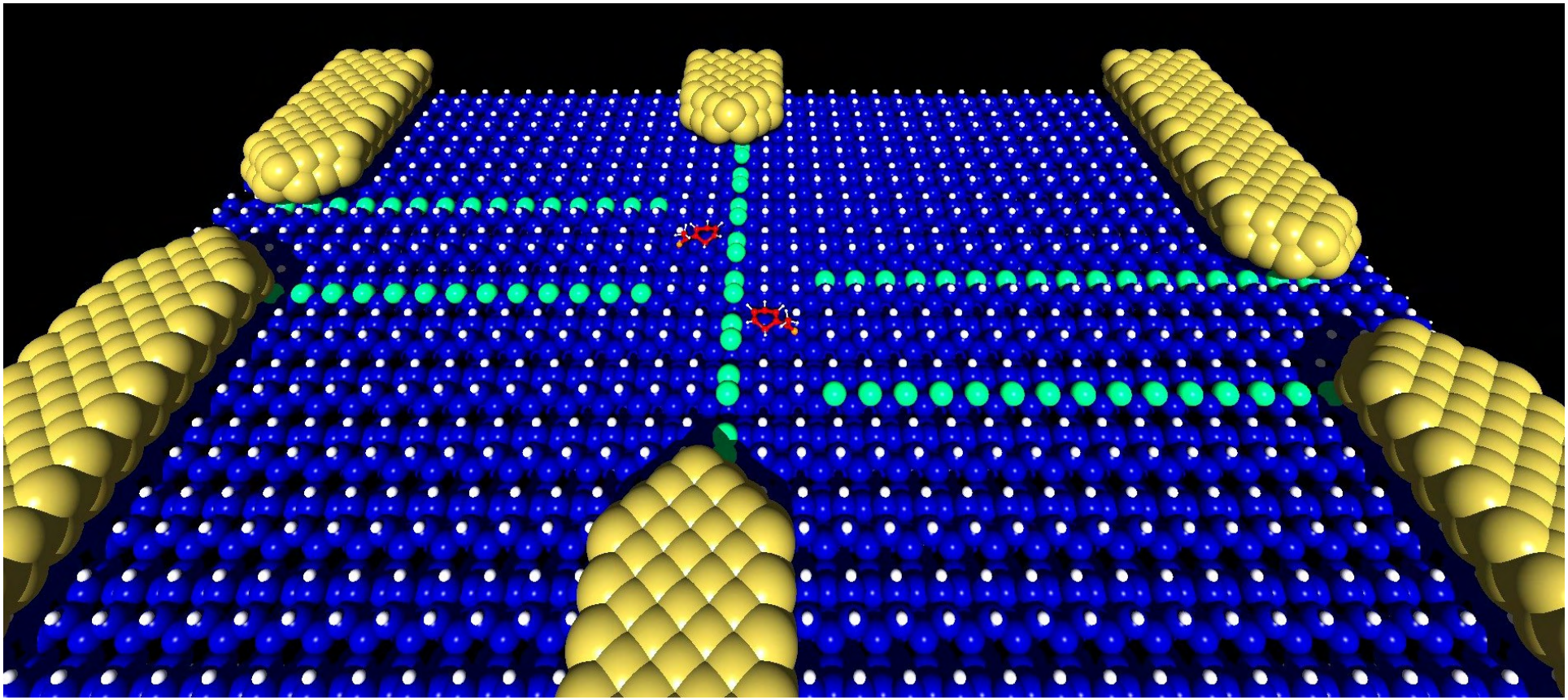
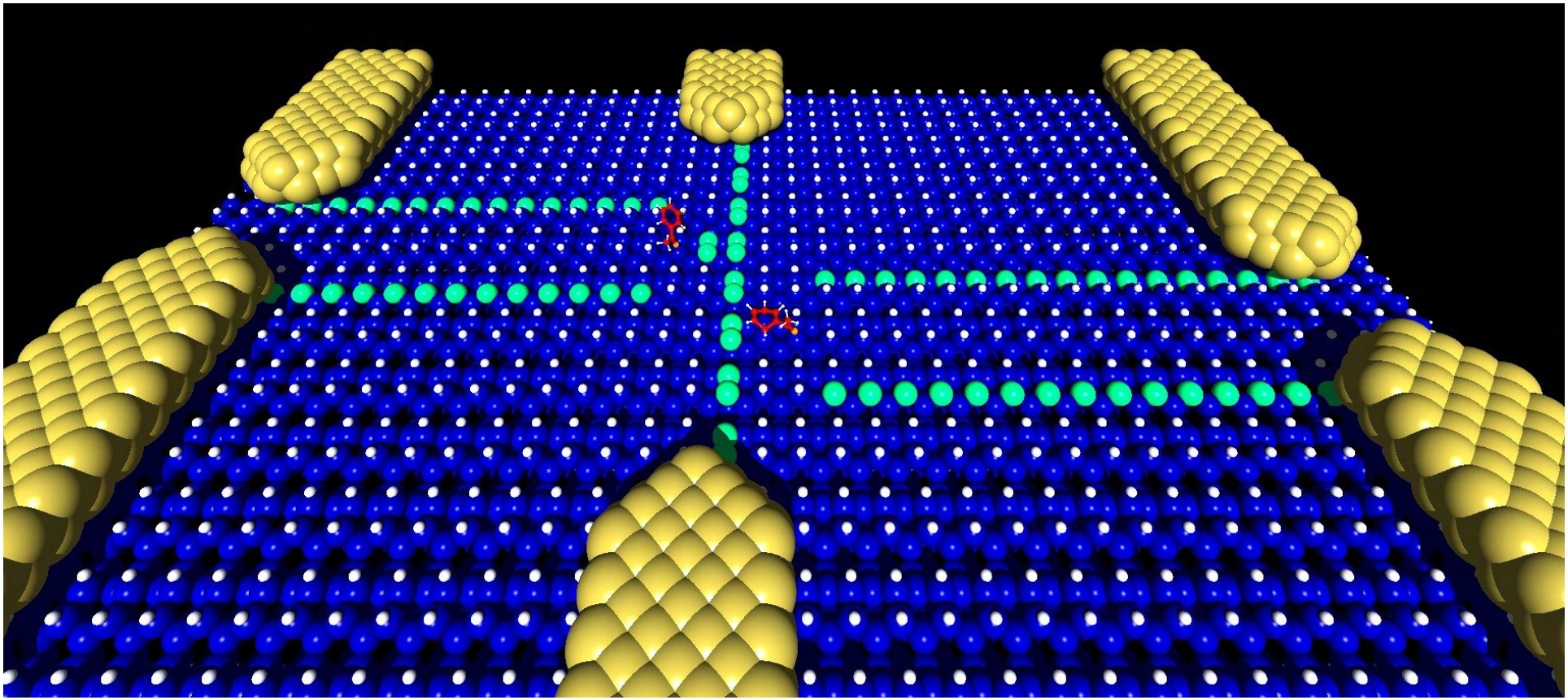


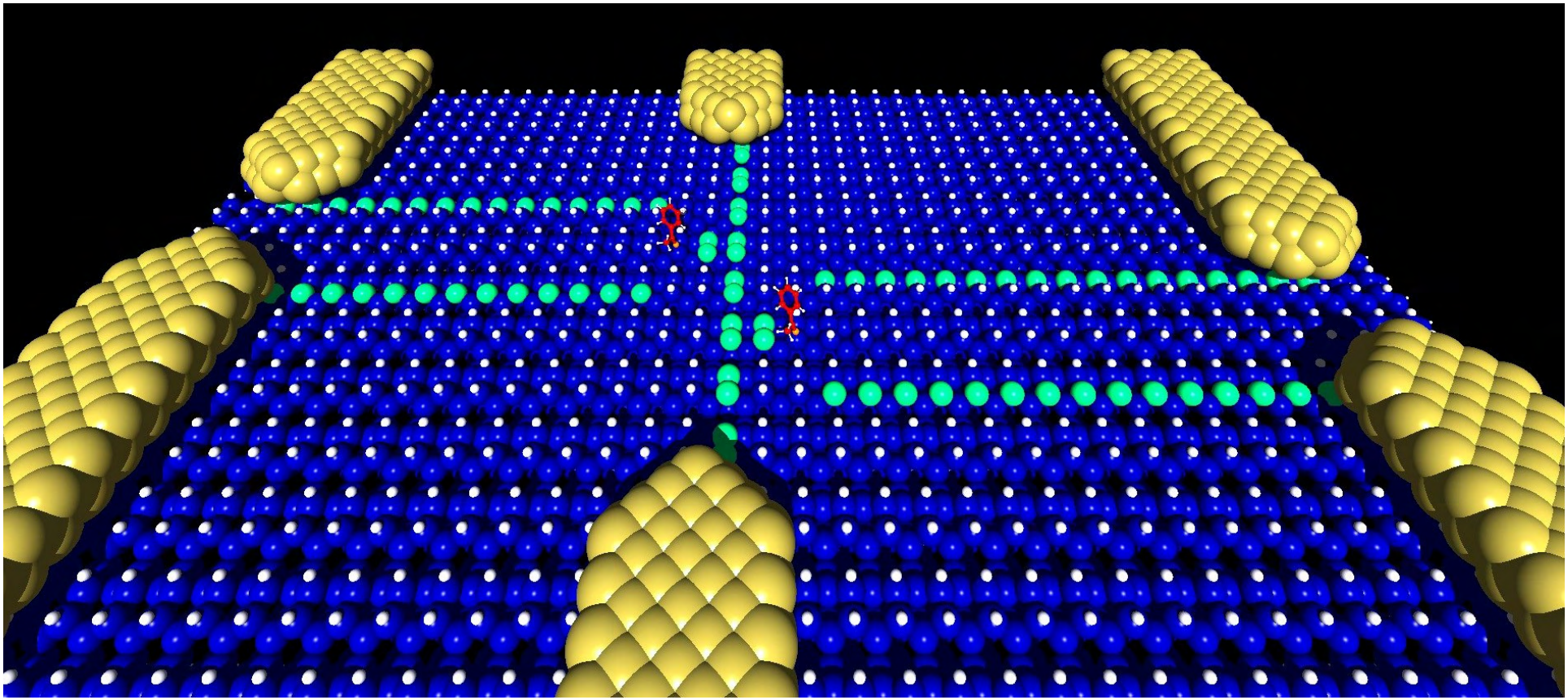


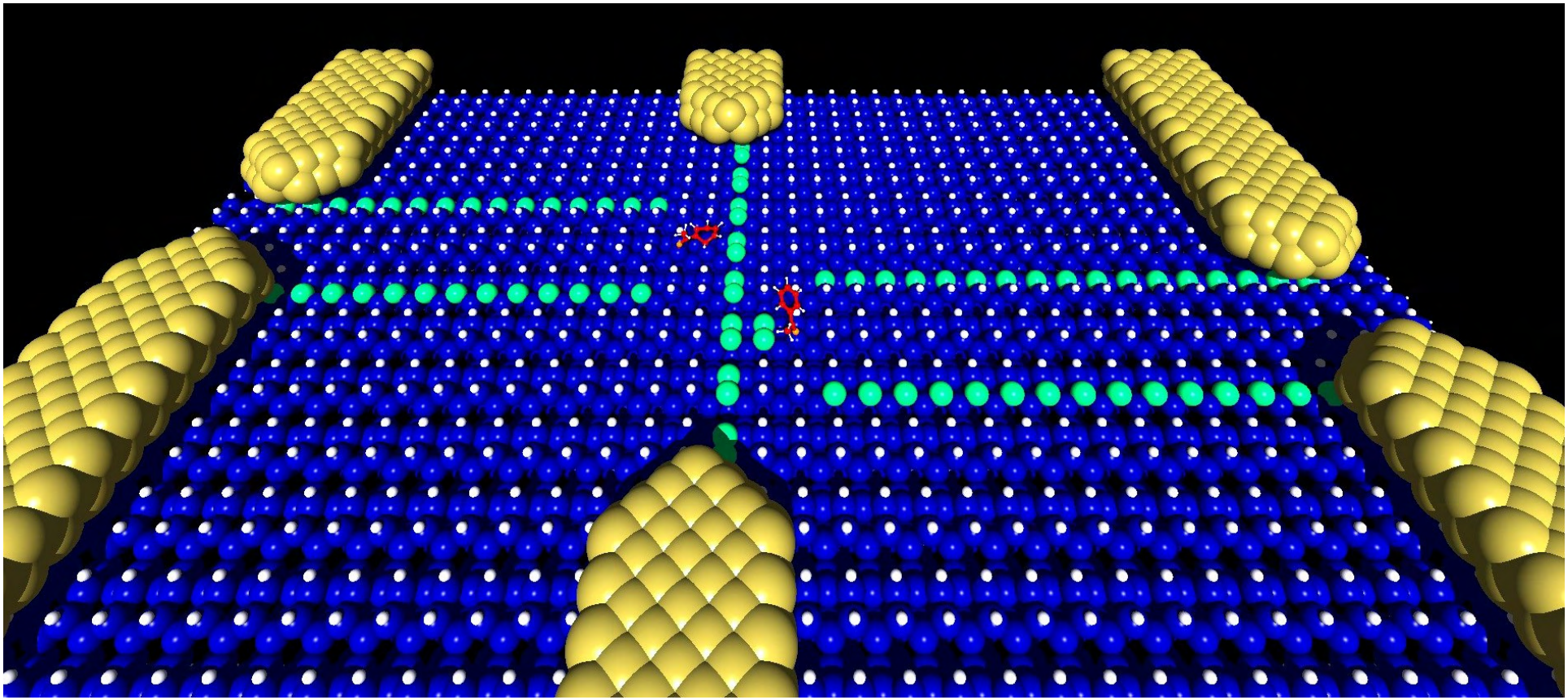




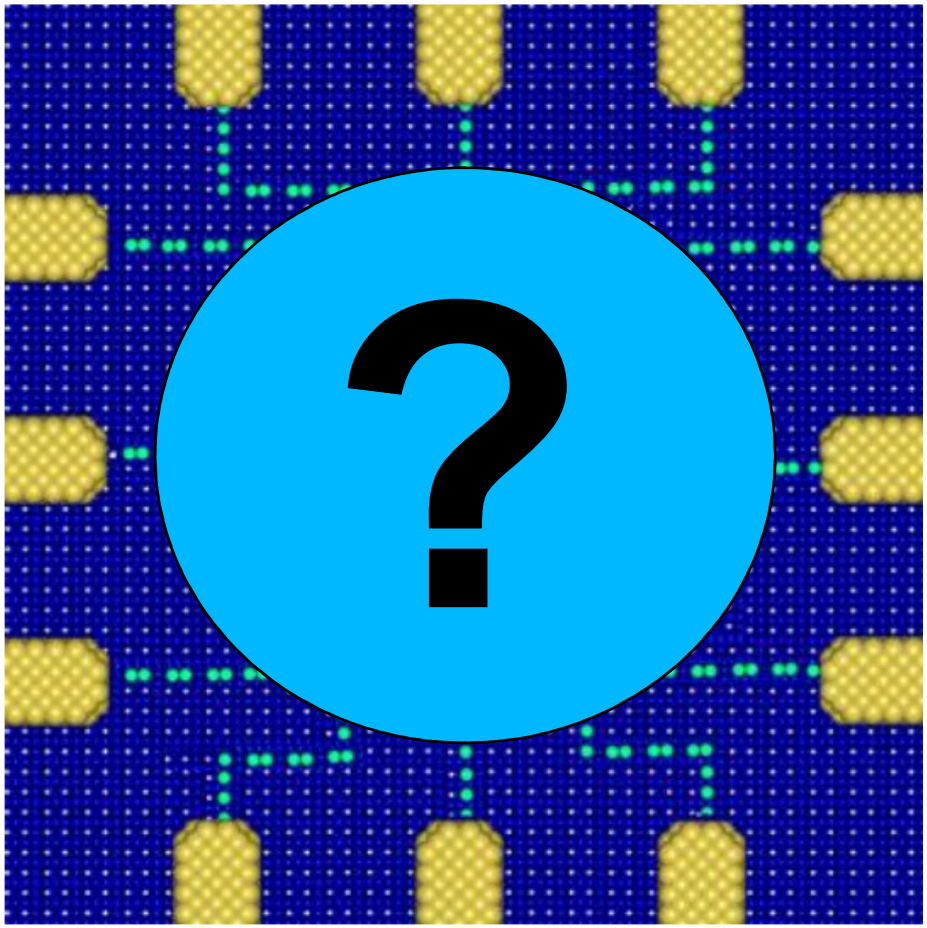








-QHC (Quantum Hamiltonian Computing) circuits



THANK YOU