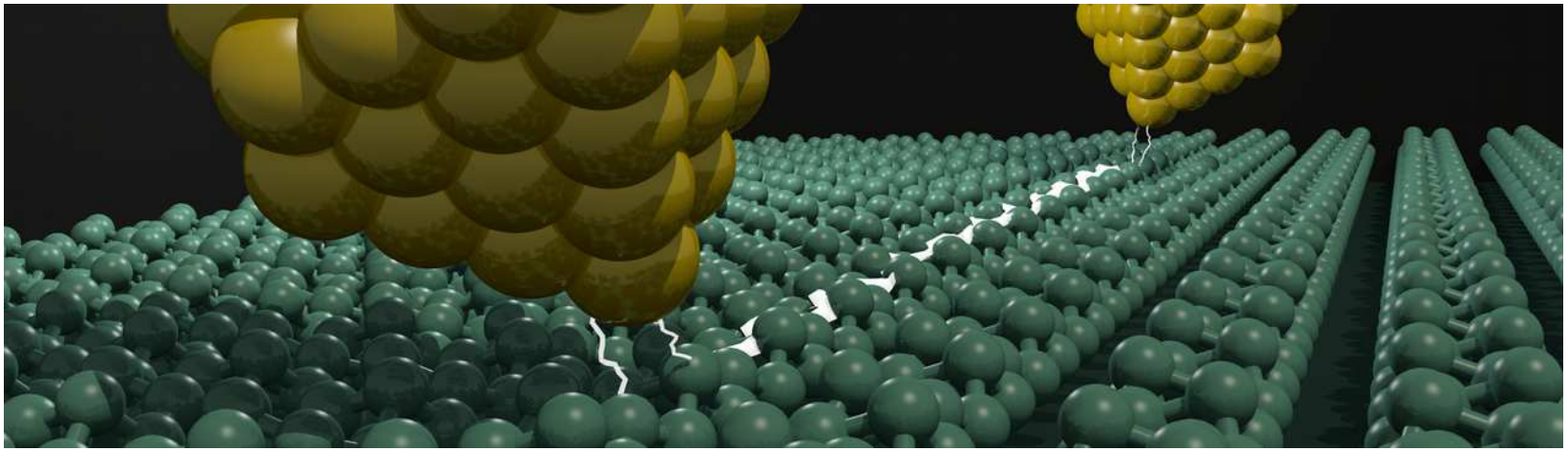
Realistic multi-terminal fist-principles transport simulations of two-probe STM measurements on Ge(001) surface: demonstration of quasi-ballistic transport through dangling-bond dimer wires

Pedro Brandimarte[1], Marek Kolmer[2,3], Hiroyo Kawai[4], Thomas Frederiksen[1,5],
brandimarte@pm.me
Aran Garcia-Lekue[1,5], Nicolas Lorente[6], Jakub Lis[2], Rafal Zuzak[2],
Szymon Godlewski[2], Christian Joachim[7], Marek Szymonski[2], Daniel Sánchez-Portal[1,6]

1 *Donostia International Physics Center, Spain*
2 *NANOSAM – Jagiellonian University, Poland*
3 *CNMS – Oak Ridge National Laboratory, USA*
4 IMRE – National University of Singapore, Singapore
5 *IKERBASQUE, Basque Foundation for Science, Spain*
6 *Centro de Física de Materiales CSIC-UPV/EHU, Spain*
7 *CEMES-CNRS, France*



M. Kolmer, P. Brandimarte* *et al. Nature Communications* **10**, 1573 (2019)

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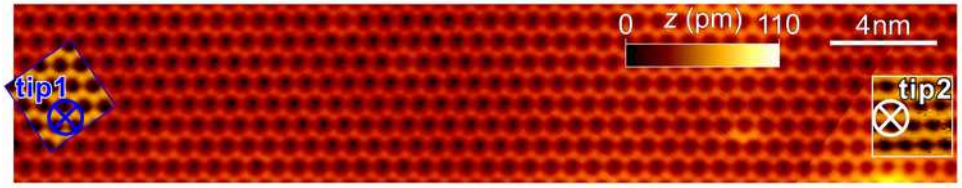
Universidad del País Vasco
Euskal Herriko Unibertsitatea
CFM
PAMS
SEVENTH FRAMEWORK PROGRAMME
GOBIERNO DE ESPAÑA
MINISTERIO DE ECONOMÍA Y COMPETITIVIDAD
CSIC
CONSEJO SUPERIOR DE INVESTIGACIONES CIENTÍFICAS

Two-probe STM at the atomic level



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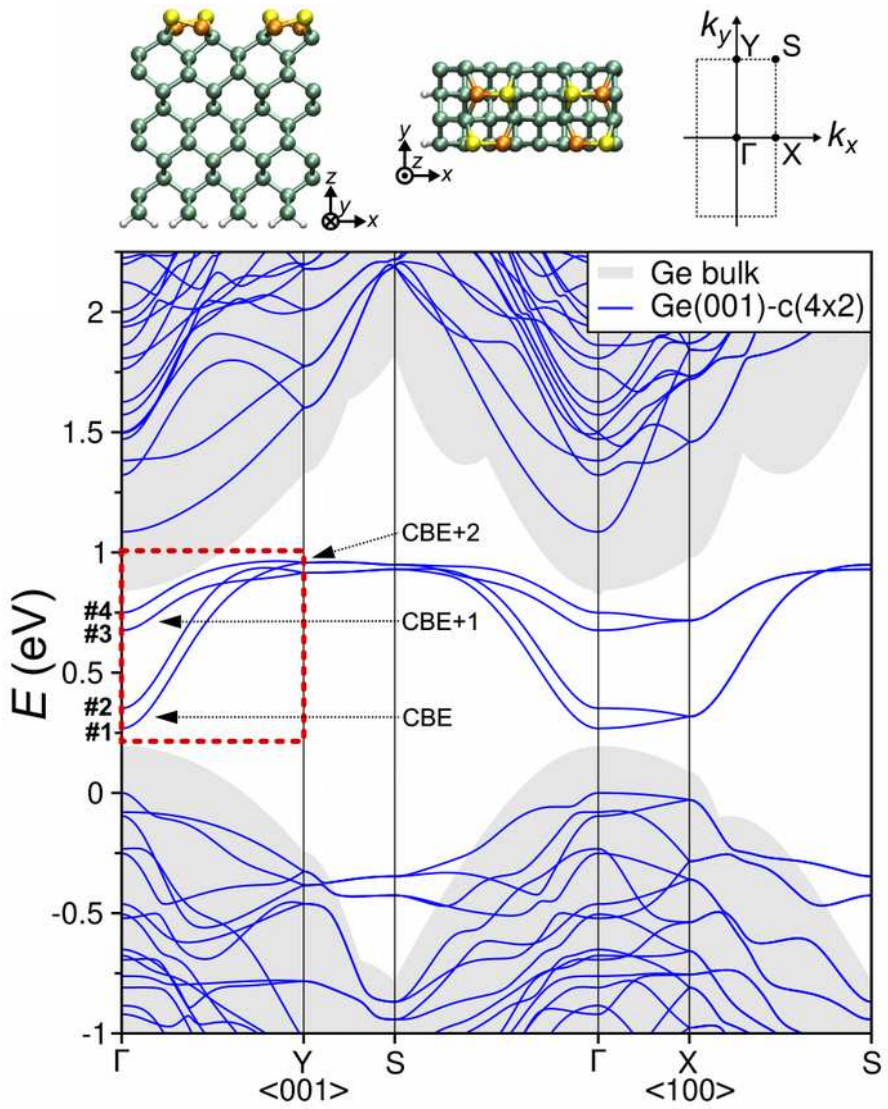
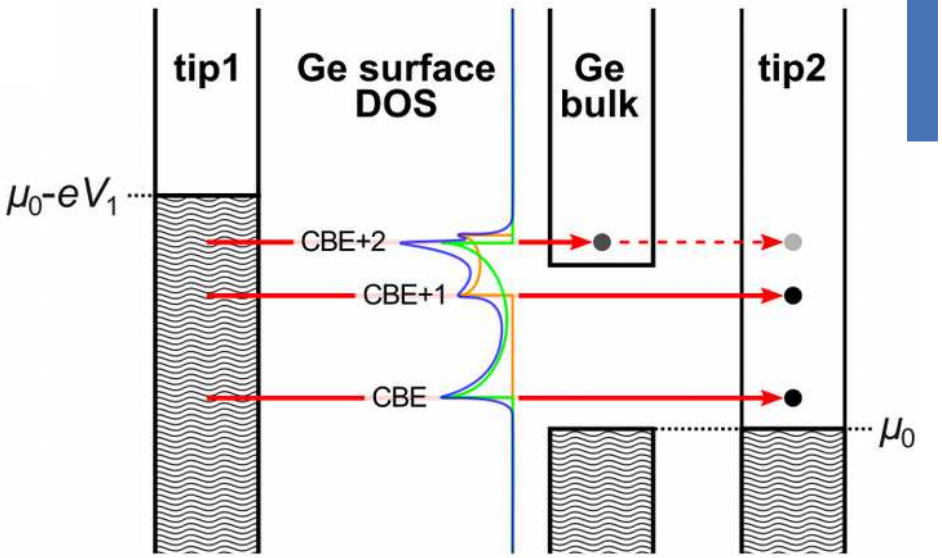
M. Kolmer *et al. J. Phys: Cond. Mat.* **29**, 444004 (2017).

Ge(001)x(4x2) surface





Methodology

Density-Functional Theory (DFT)

+

Non-Equilibrium Green's Function (NEGF)

TranSIESTA

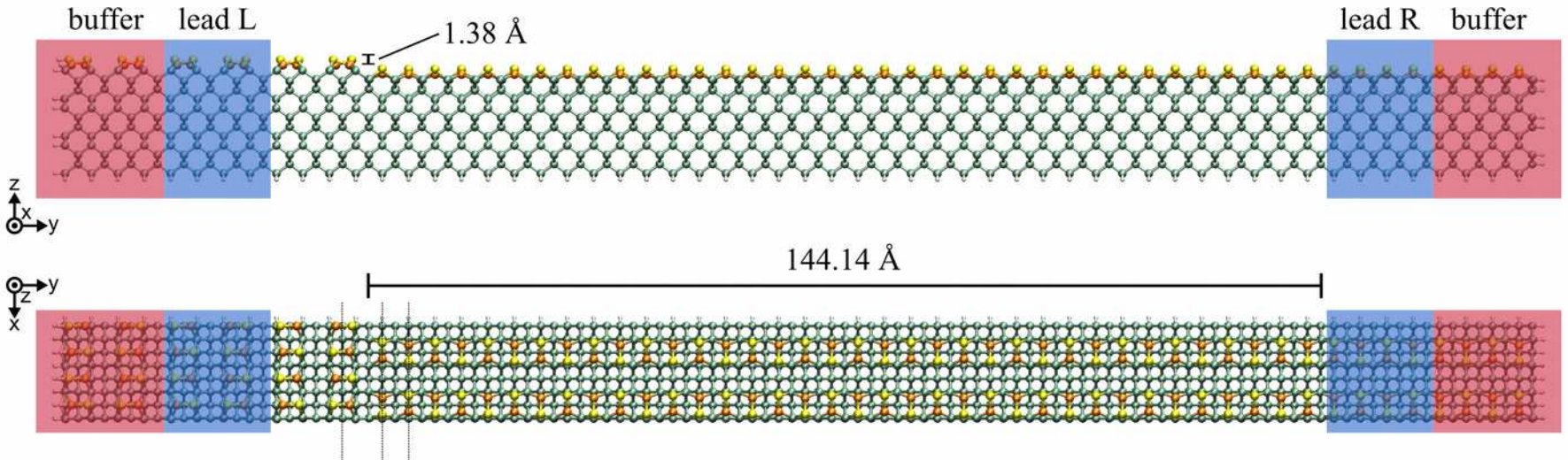
E. Artacho *et al*. *Phys. Stat. Sol.* (b) **215**, 809 (1999).

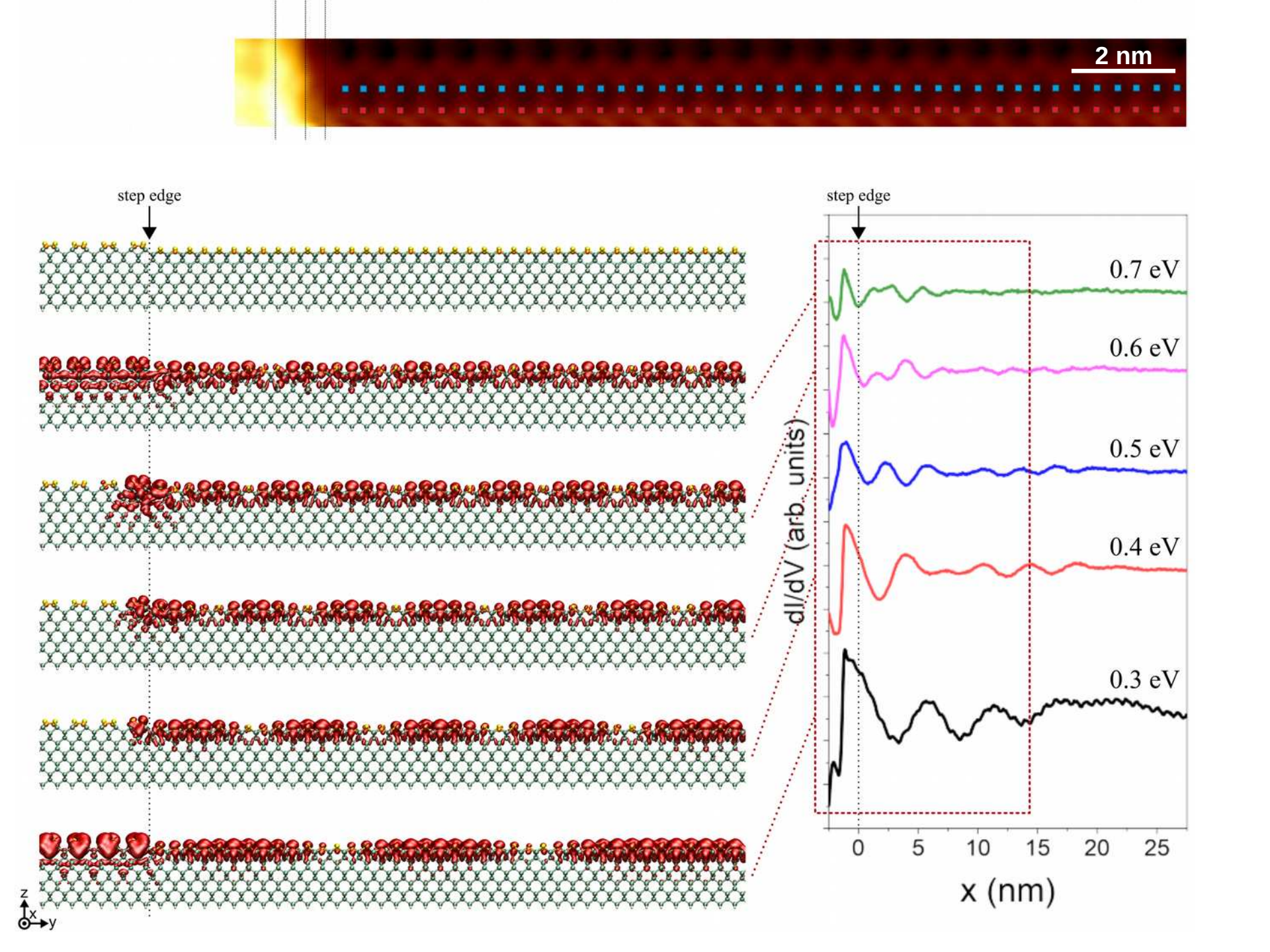
J. M. Soler *et al*. *J. Phys. Condens. Matter.* **14**, 2745 (2002).

M. Brandbyge *et al*. *Phys. Rev. B* **65**, 165401 (2002).

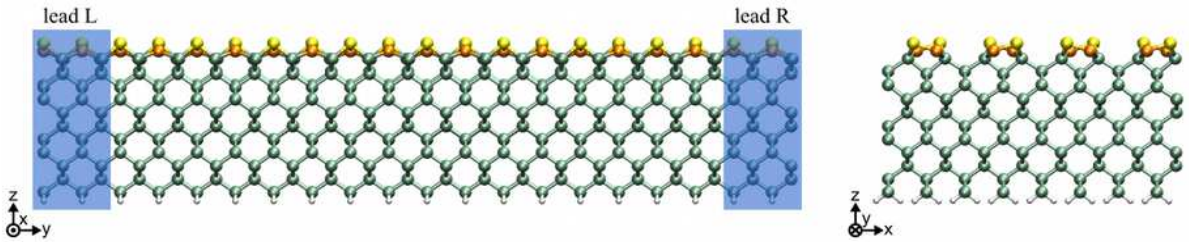
N. Papior *et al*. *Comp. Phys. Comm.* **212**, 8 (2017).

Ge(001) step edge: coherence length



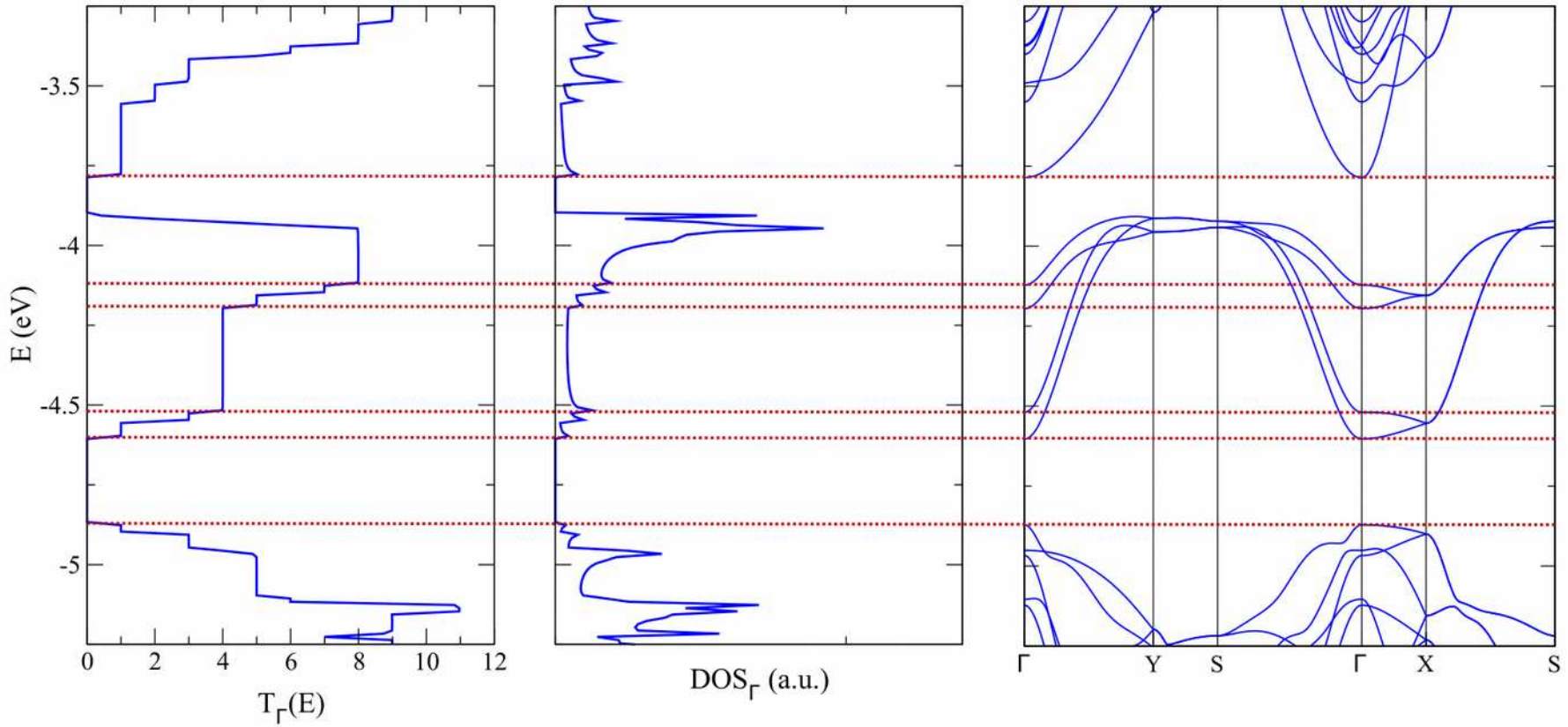

2 nm
step edge
step edge
0.7 eV
0.6 eV
0.5 eV
0.4 eV
0.3 eV
dI/dV (arb. units)
0
5
10
15
20
25
x (nm)
z
x
y

Ge(001) surface: 2-terminal setup

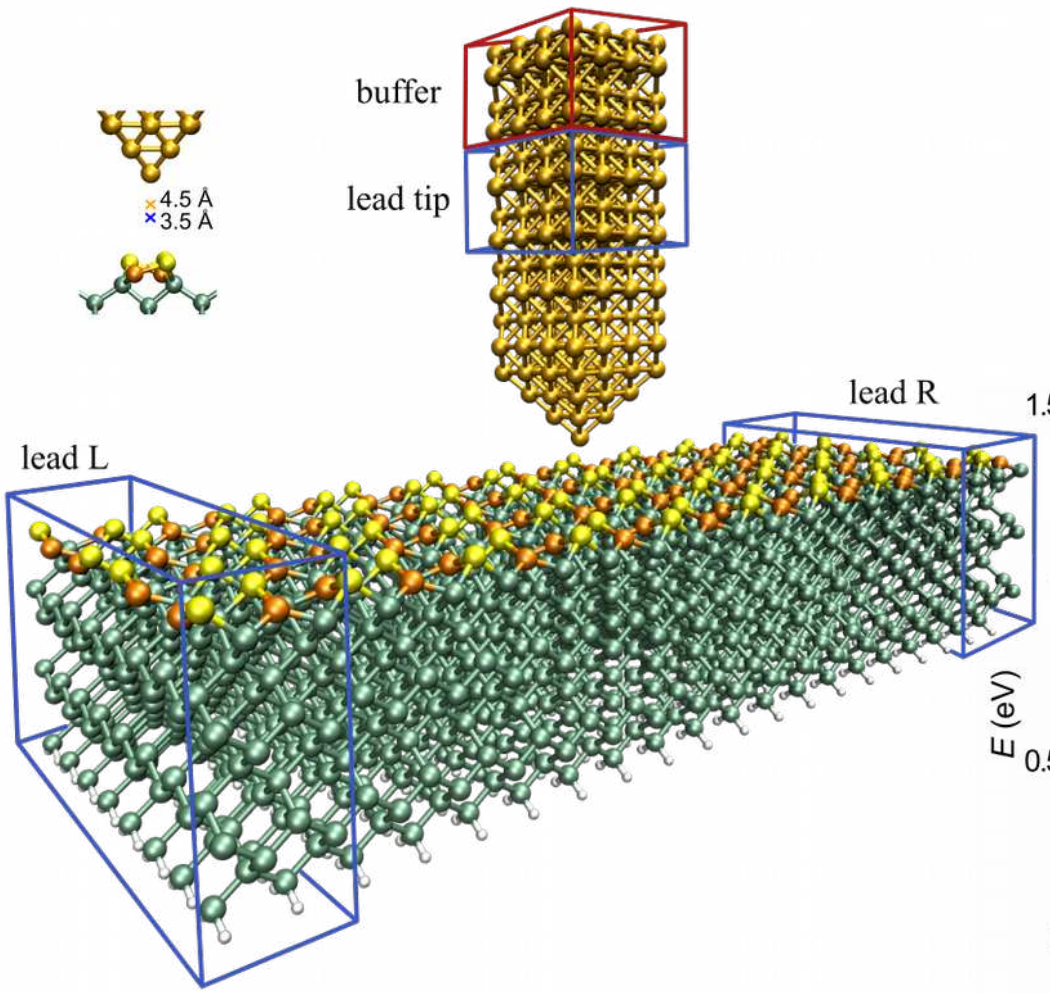


Simulation characteristics:

- # of atoms/orbitals: **2240/16000**
- cell size: **32.03x80.07x34 Å^3**

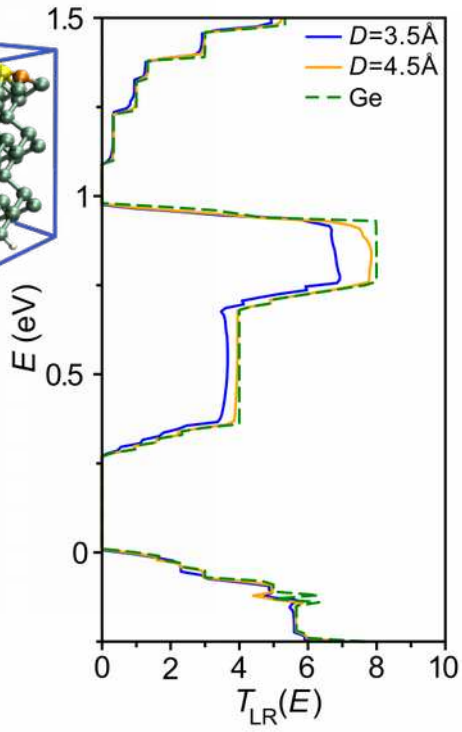


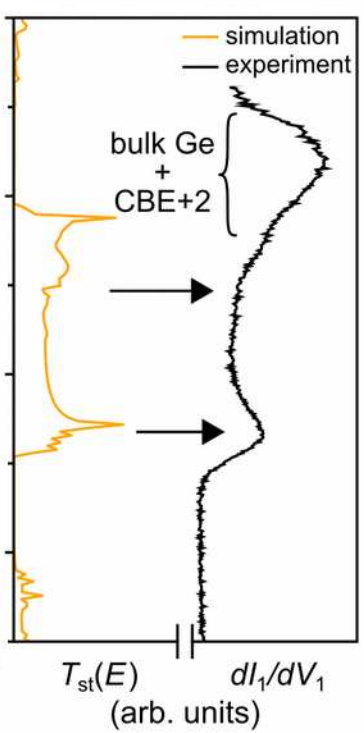
Ge(001) surface addressed by a single tip: 3-terminal setup



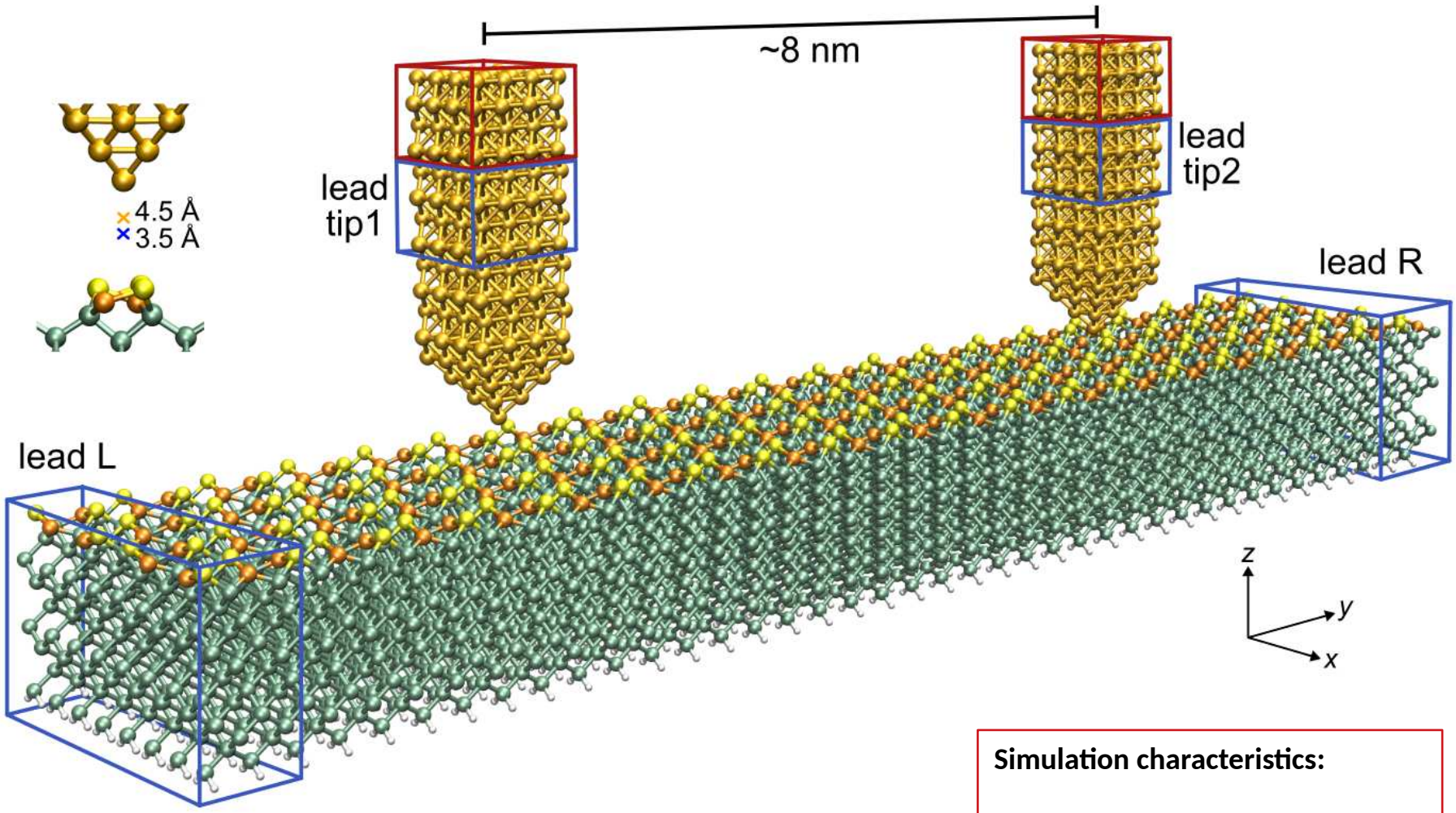
Simulation characteristics:

- # of atoms/orbitals: **2462/18221**
- cell size: **32.03x80.07x80 Å^3**



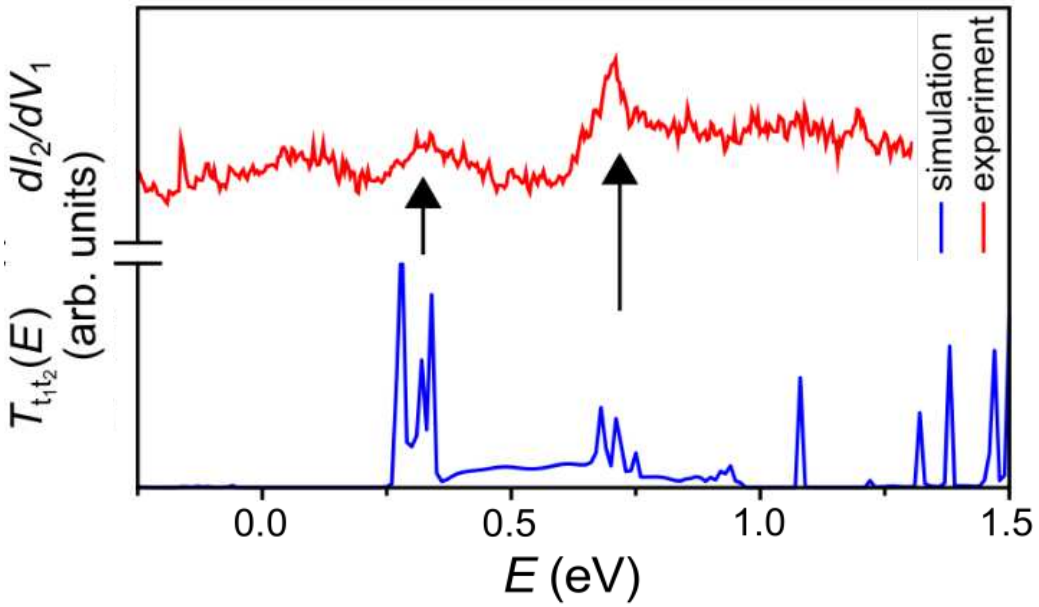


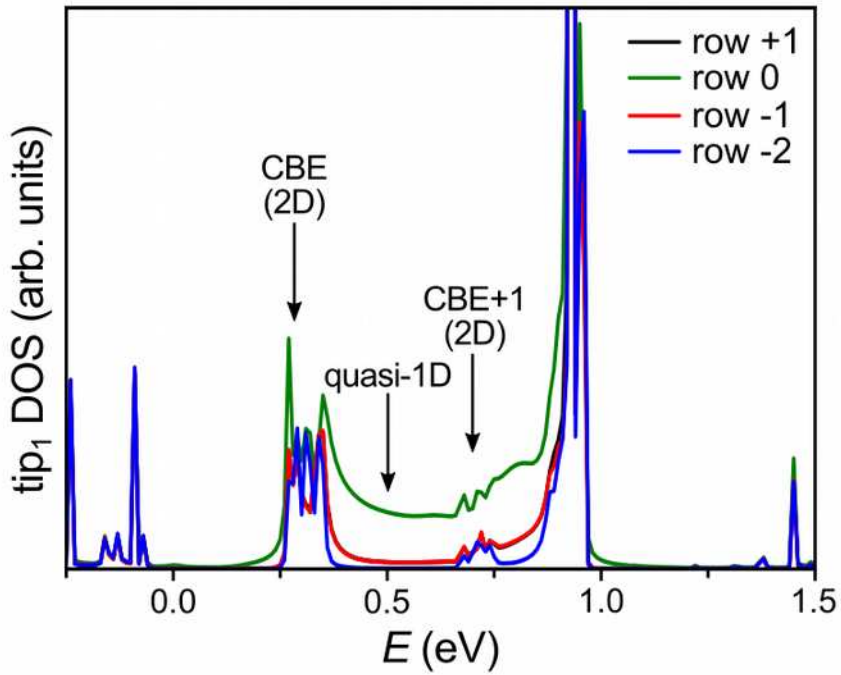
Ge(001) surface addressed by two tips: 4-terminal setup

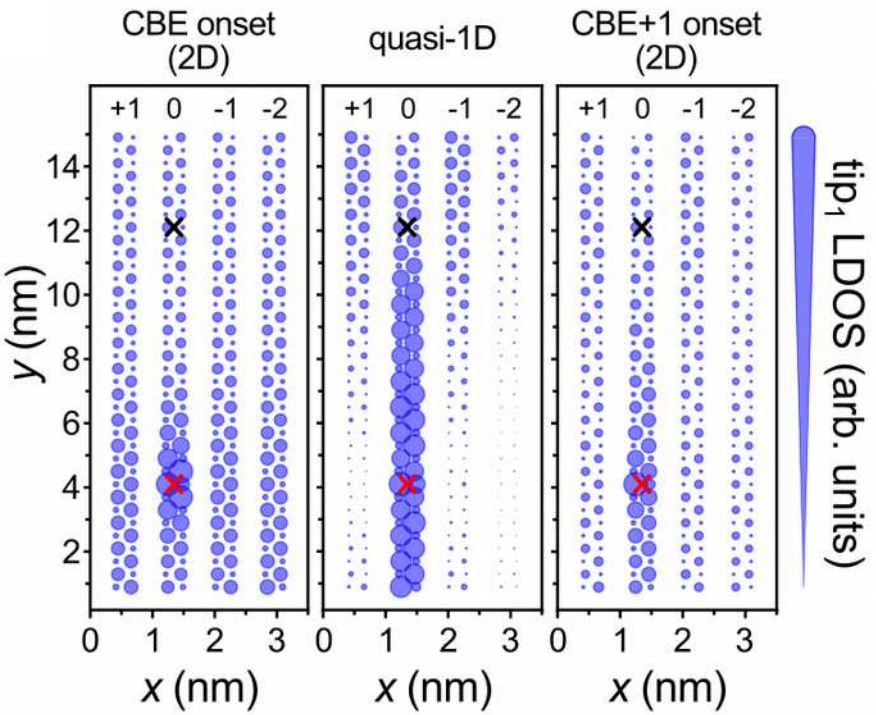


Simulation characteristics:

- # of atoms/orbitals: **4924/36442**
- cell size: **32.03x160.15x80 Å^3**


dI_2/dV_1
$T_{t_1t_2}(E)$ (arb. units)
simulation
experiment
0.0
0.5
1.0
1.5
E (eV)


tip$_1$ DOS (arb. units)
row +1
row 0
row -1
row -2
CBE
(2D)
quasi-1D
CBE+1
(2D)
0.0
0.5
1.0
1.5
E (eV)


CBE onset
(2D)
quasi-1D
CBE+1 onset
(2D)
+1
0
-1
-2
y (nm)
2
4
6
8
10
12
14
0
1
2
3
x (nm)
tip$_1$ LDOS (arb. units)