



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 Brandimarte¹, Marek Kolmer², Hiroyo Kawai³, Thomas Frederiksen^{1,4},
Aran Garcia-Lekue^{1,4}, Nicolas Lorente⁵, Mads Engelund⁵, Rafal Zuzak²,
Szymon Godlewski², Christian Joachim⁶, Marek Szymonski², Daniel Sánchez-Portal^{1,5}

¹ Donostia International Physics Center, Spain

² NANOSAM - Jagiellonian University, Poland

³ IMRE - National University of Singapore, Singapore

⁴ IKERBASQUE, Basque Foundation for Science, Spain

⁵ Centro de Física de Materiales CSIC-UPV/EHU, Spain

⁶ CEMES-CNRS, France

May 10, 2018



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 Brandimarte¹, Marek Kolmer², Hiroyo Kawai³, Thomas Frederiksen^{1,4},
Aran Garcia-Lekue^{1,4}, Nicolas Lorente⁵, Mads Engelund⁵, Rafal Zuzak²,
Szymon Godlewski², Christian Joachim⁶, Marek Szymonski², Daniel Sánchez-Portal^{1,5}

1 Donostia International Physics Center, Spain

2 NANOSAM - Jagiellonian University, Poland

3 IMRE - National University of Singapore, Singapore

4 IKERBASQUE, Basque Foundation for Science, Spain

5 Centro de Física de Materiales CSIC-UPV/EHU, Spain

6 CEMES-CNRS, France

May 10, 2018



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 Brandimarte¹, Marek Kolmer², Hiroyo Kawai³, Thomas Frederiksen^{1,4},
Aran Garcia-Lekue^{1,4}, Nicolas Lorente⁵, Mads Engelund⁵, Rafal Zuzak²,
Szymon Godlewski², Christian Joachim⁶, Marek Szymonski², Daniel Sánchez-Portal^{1,5}

1 Donostia International Physics Center, Spain

2 NANOSAM - Jagiellonian University, Poland

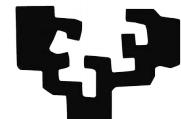
3 IMRE - National University of Singapore, Singapore

4 IKERBASQUE, Basque Foundation for Science, Spain

5 Centro de Física de Materiales CSIC-UPV/EHU, Spain

6 CEMES-CNRS, France

May 10, 2018



Two-probe STM at the atomic level



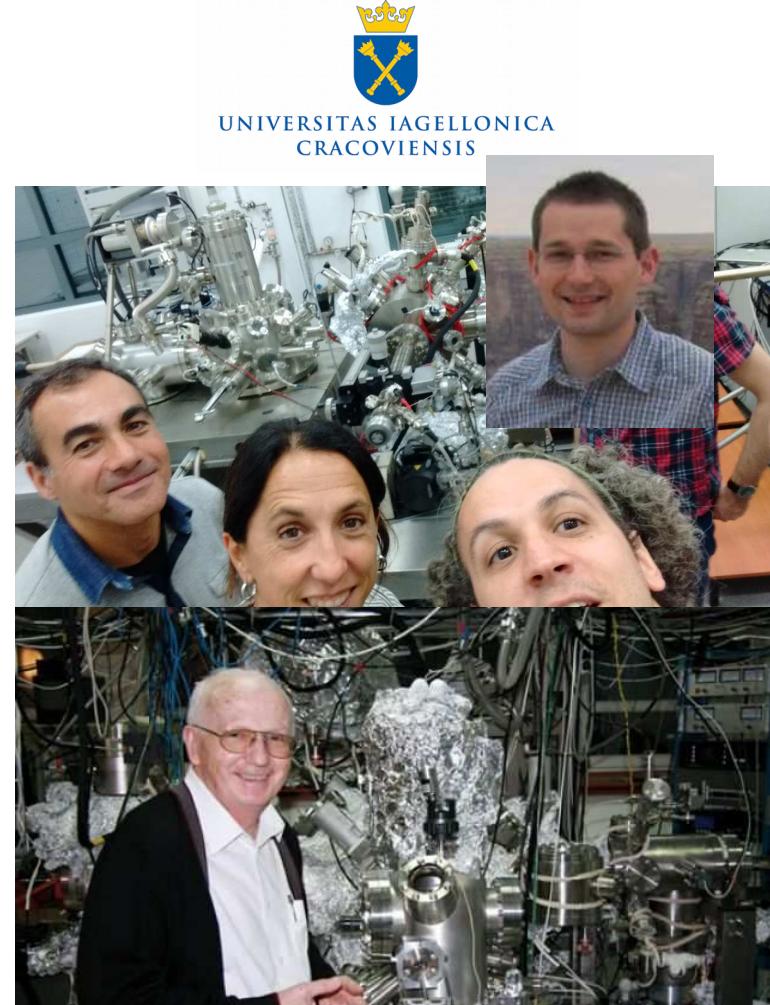


Two-probe STM at the atomic level





Two-probe STM at the atomic level



Methods

Density-Functional Theory (DFT)

+

Non-Equilibrium Green's Function (NEGF)

SIESTA

E. Artacho *et al.* *Phys. Stat. Sol. (b)* **215**, 809 (1999).
J. M. Soler *et al.* *J. Phys. Condens. Matter.* **14**, 2745 (2002).

Methods

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).

Methods

Density-Functional Theory (DFT)

+

Non-Equilibrium Green's Function (NEGF)

TranSIESTA

Multi-terminal!!!

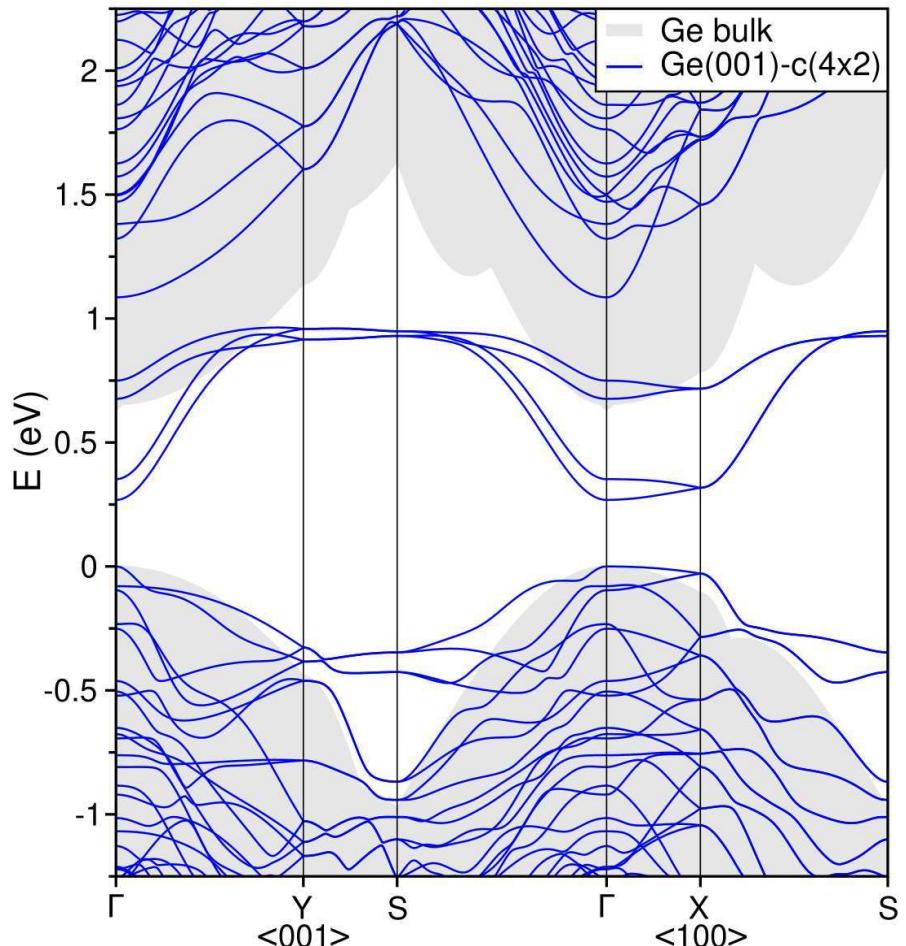
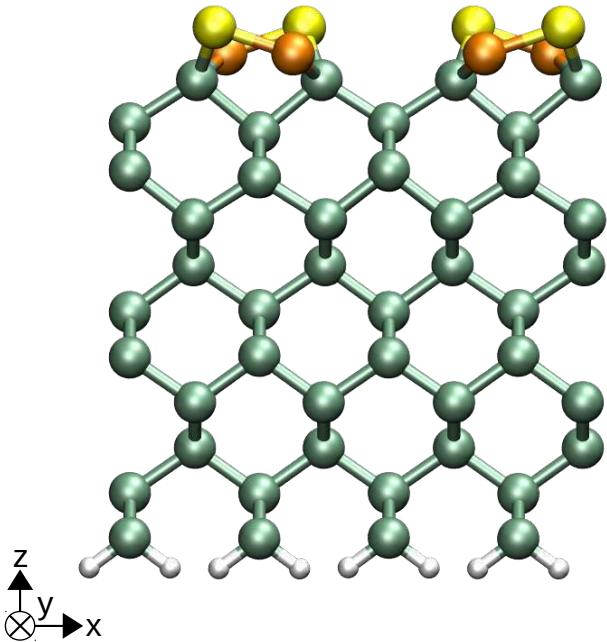
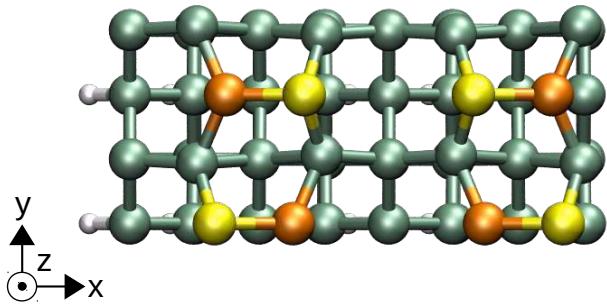
E. Artacho *et al.* Phys. Stat. Sol. (b) **215**, 809 (1999).

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

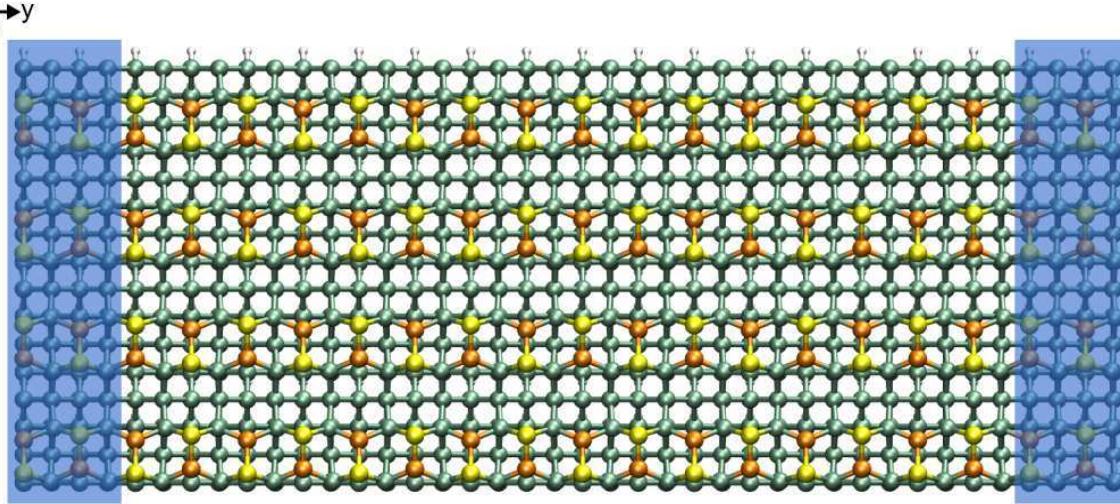
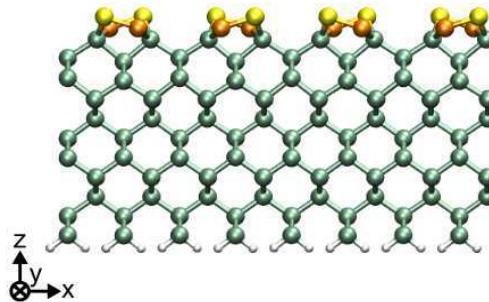
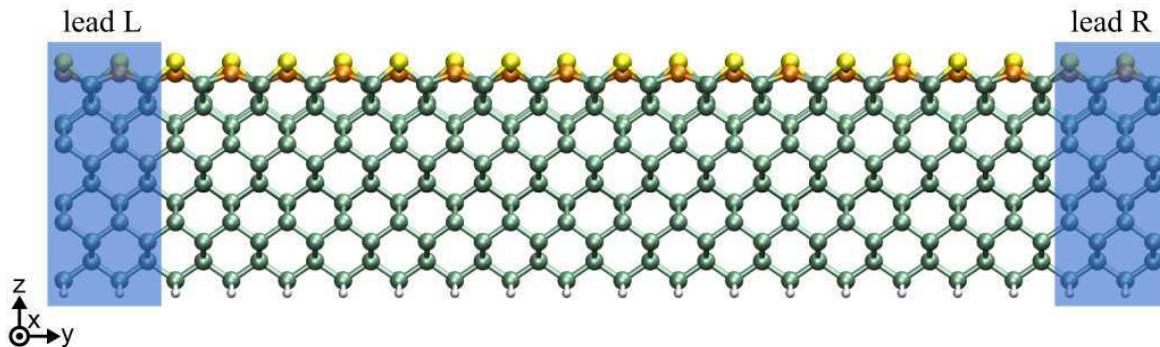
M. Brandbyge *et al.* Phys. Rev. B **65**, 165401 (2002).

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

Ge(001)x(4x2) surface



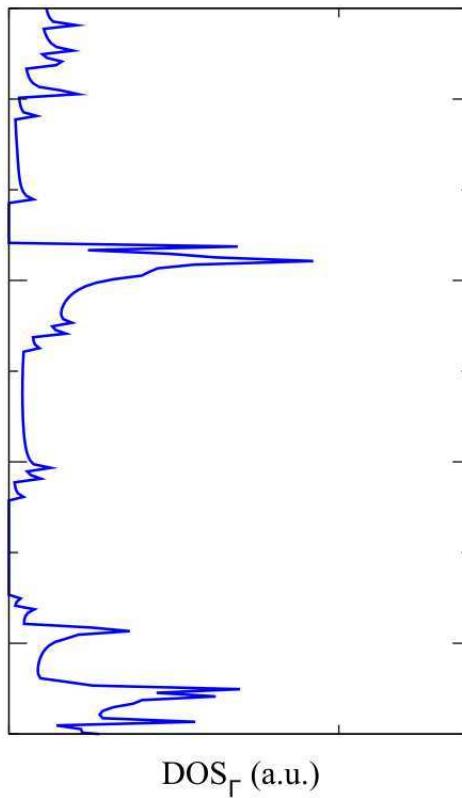
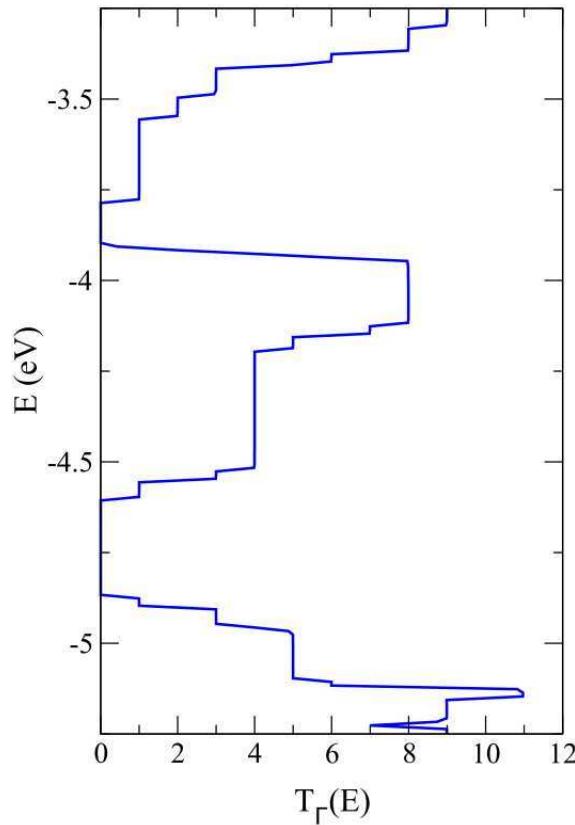
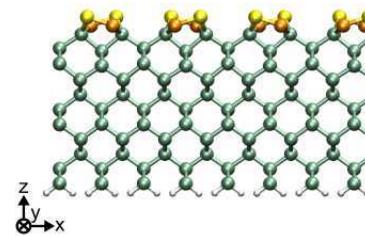
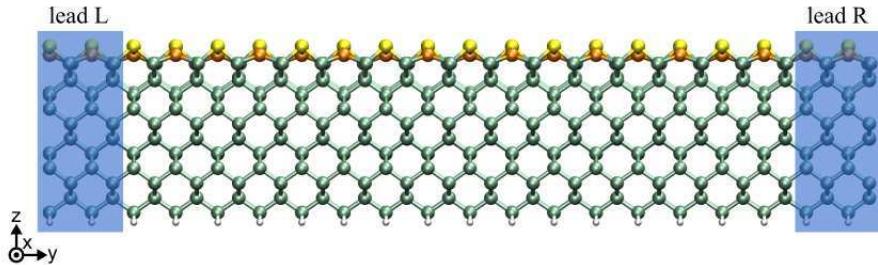
Ge(001) surface: 2-terminal setup



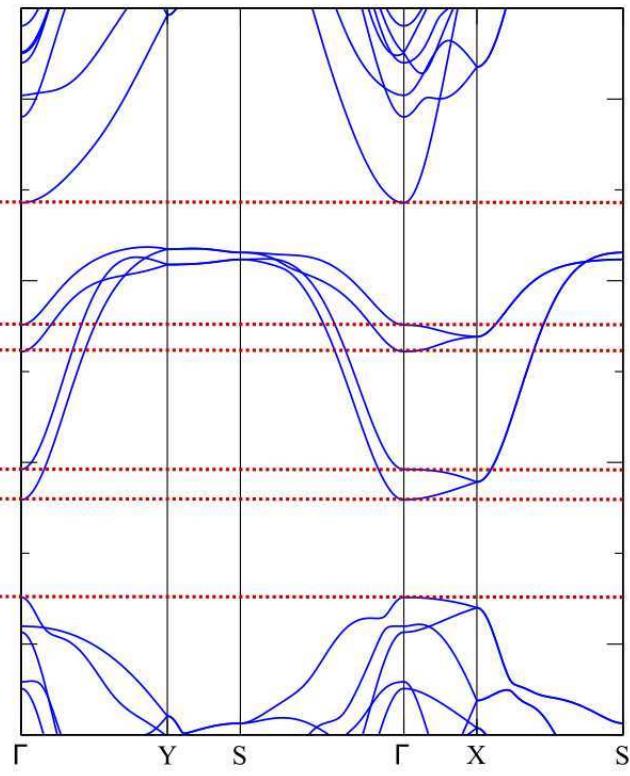
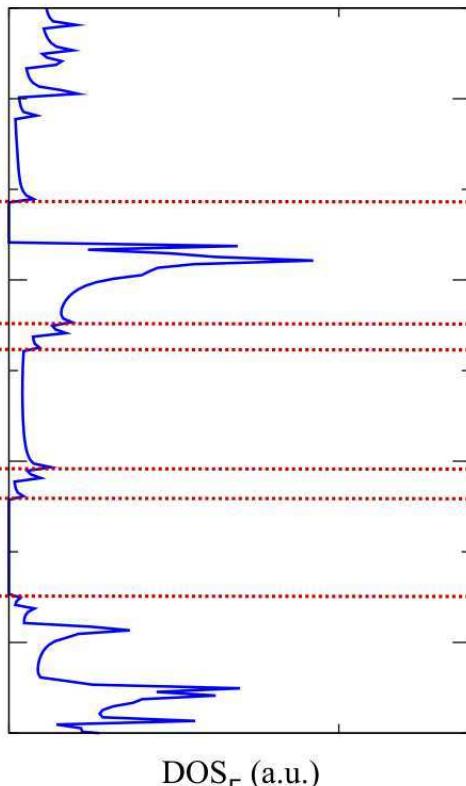
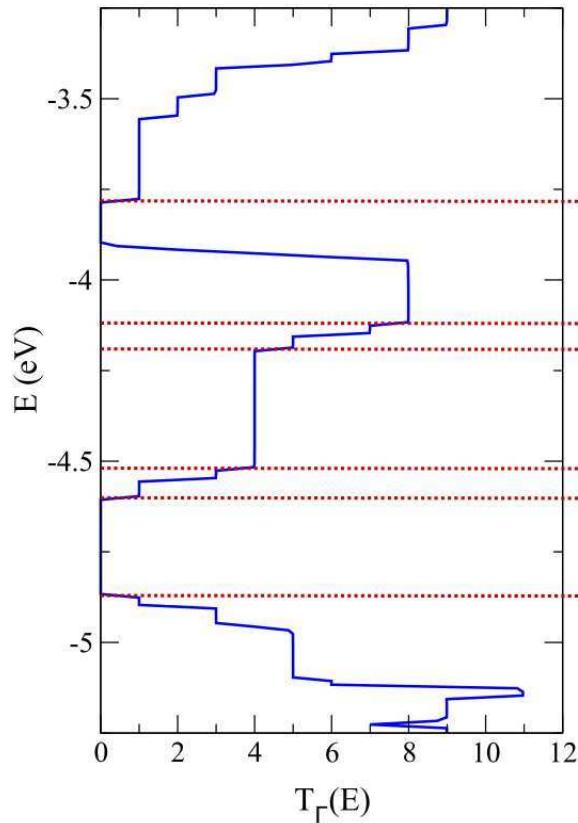
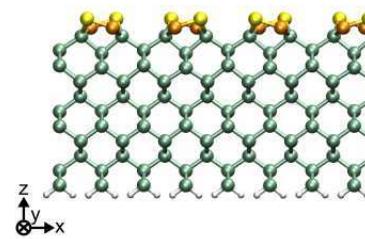
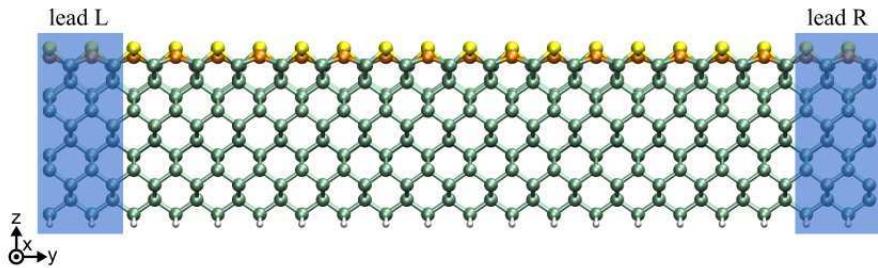
Simulation characteristics:

- # of atoms/orbitals: 2240/16000
- cell size: 32.03x80.07x34 Å³

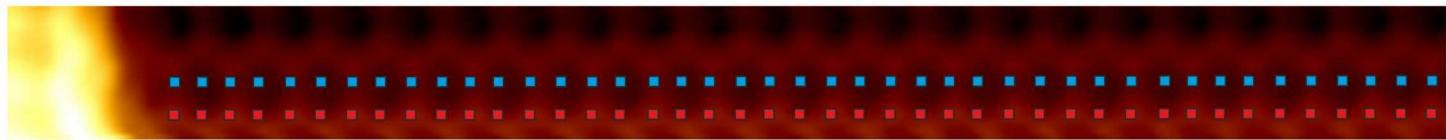
Ge(001) surface: 2-terminal setup



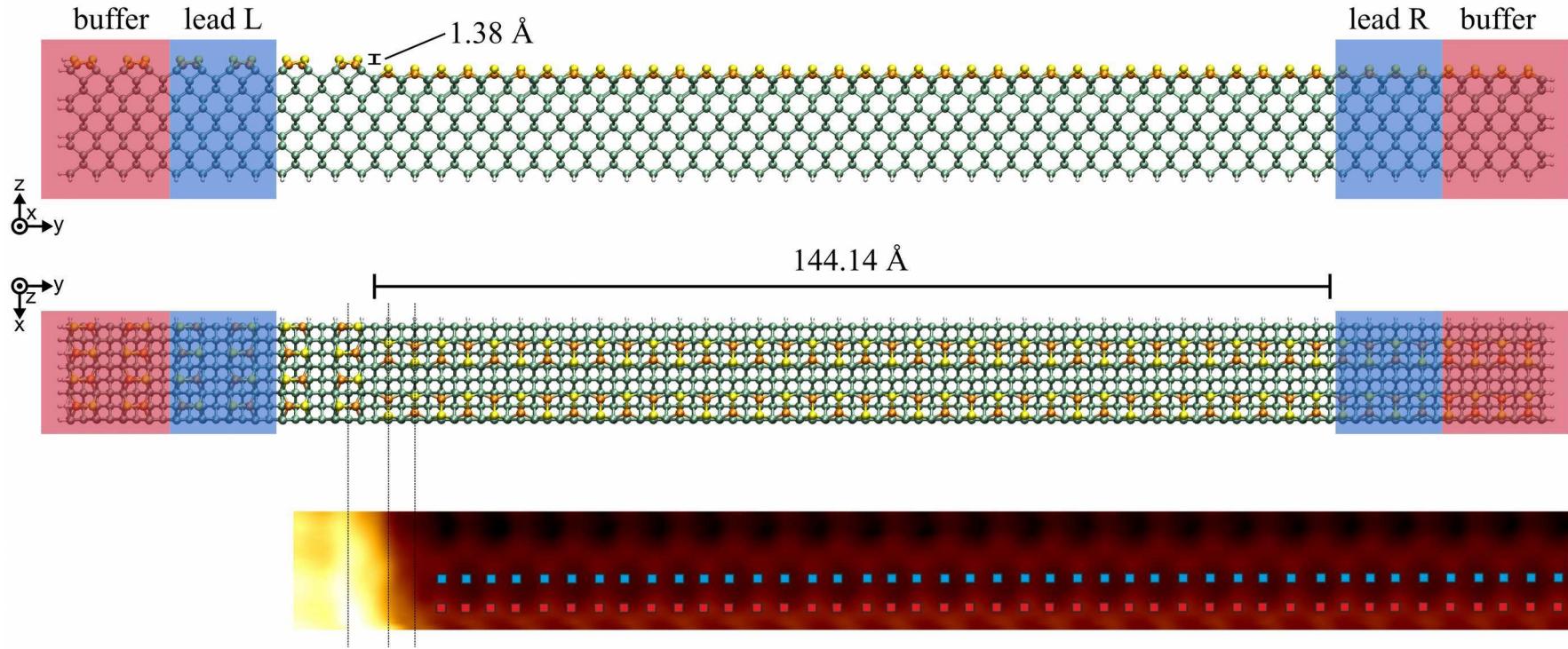
Ge(001) surface: 2-terminal setup



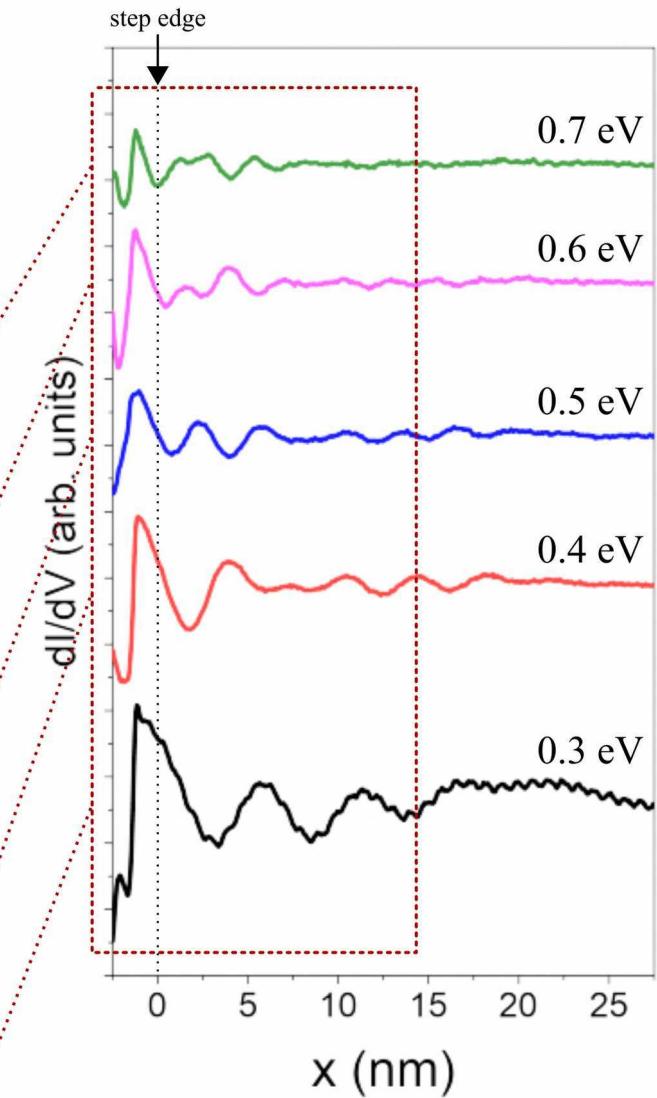
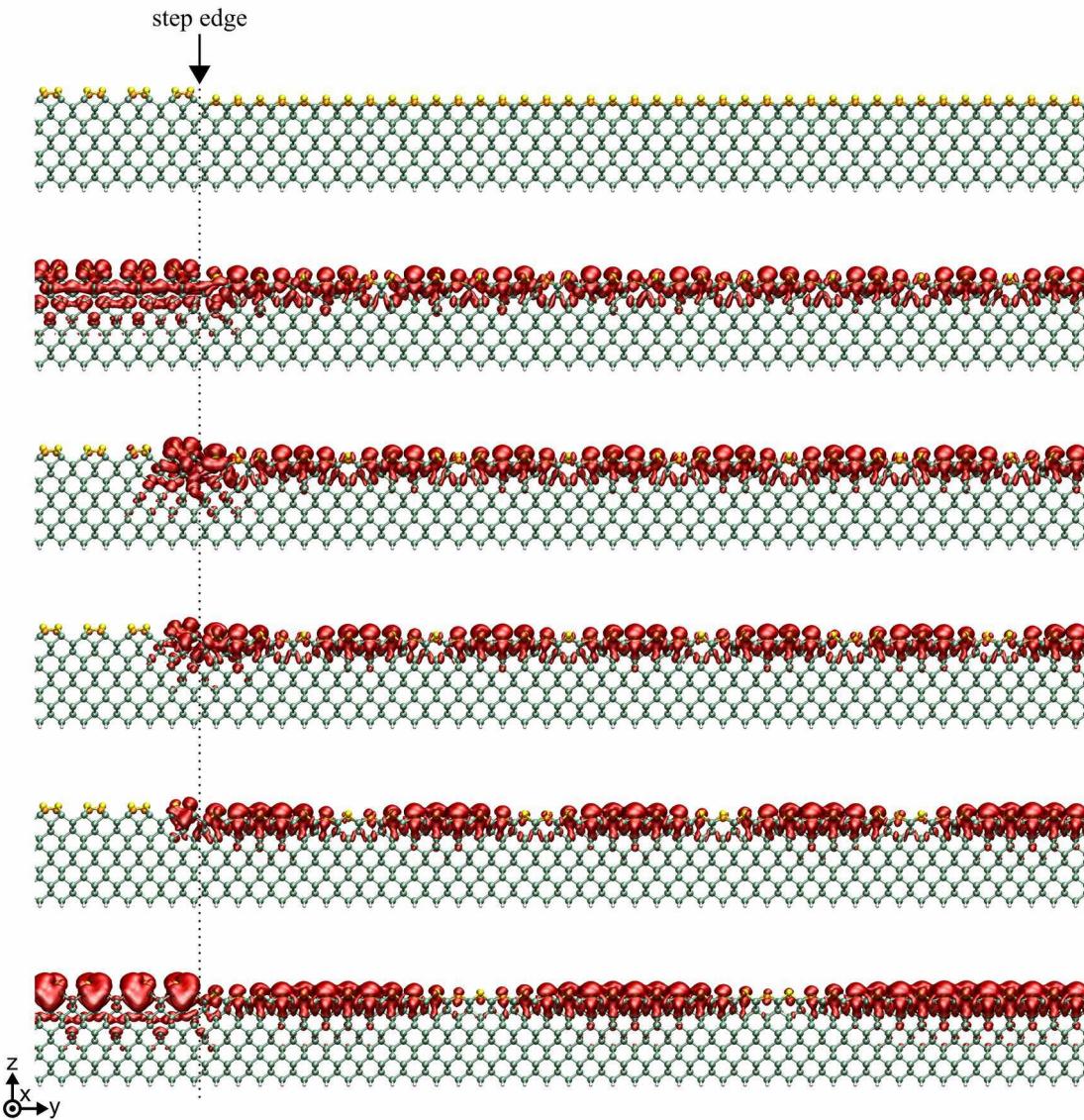
Ge(001) step edge: coherence length



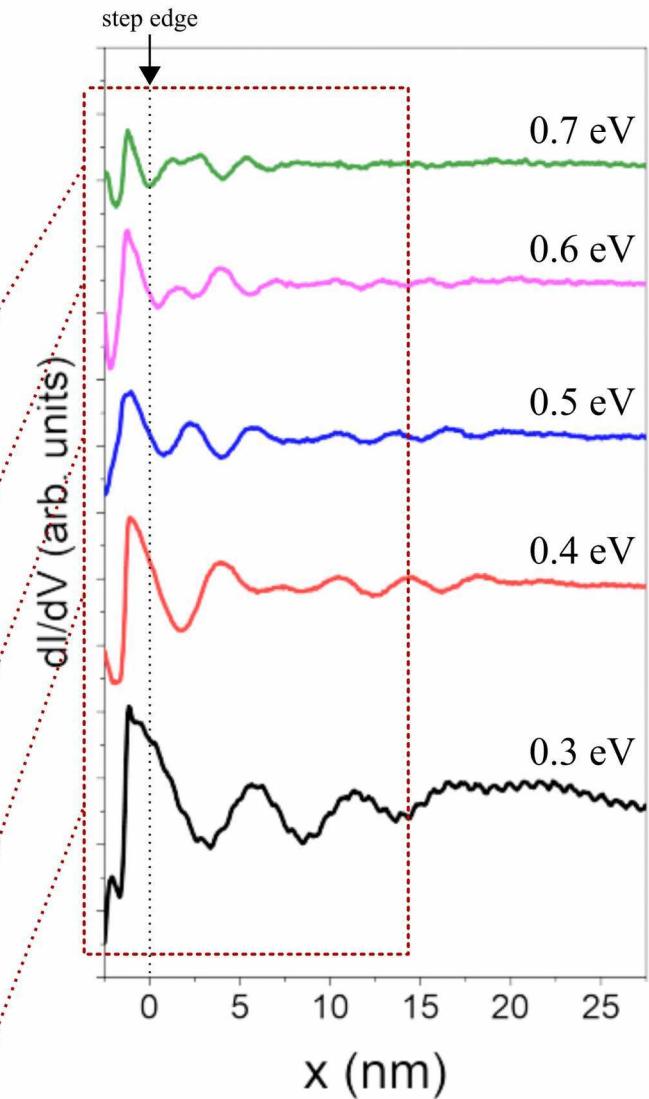
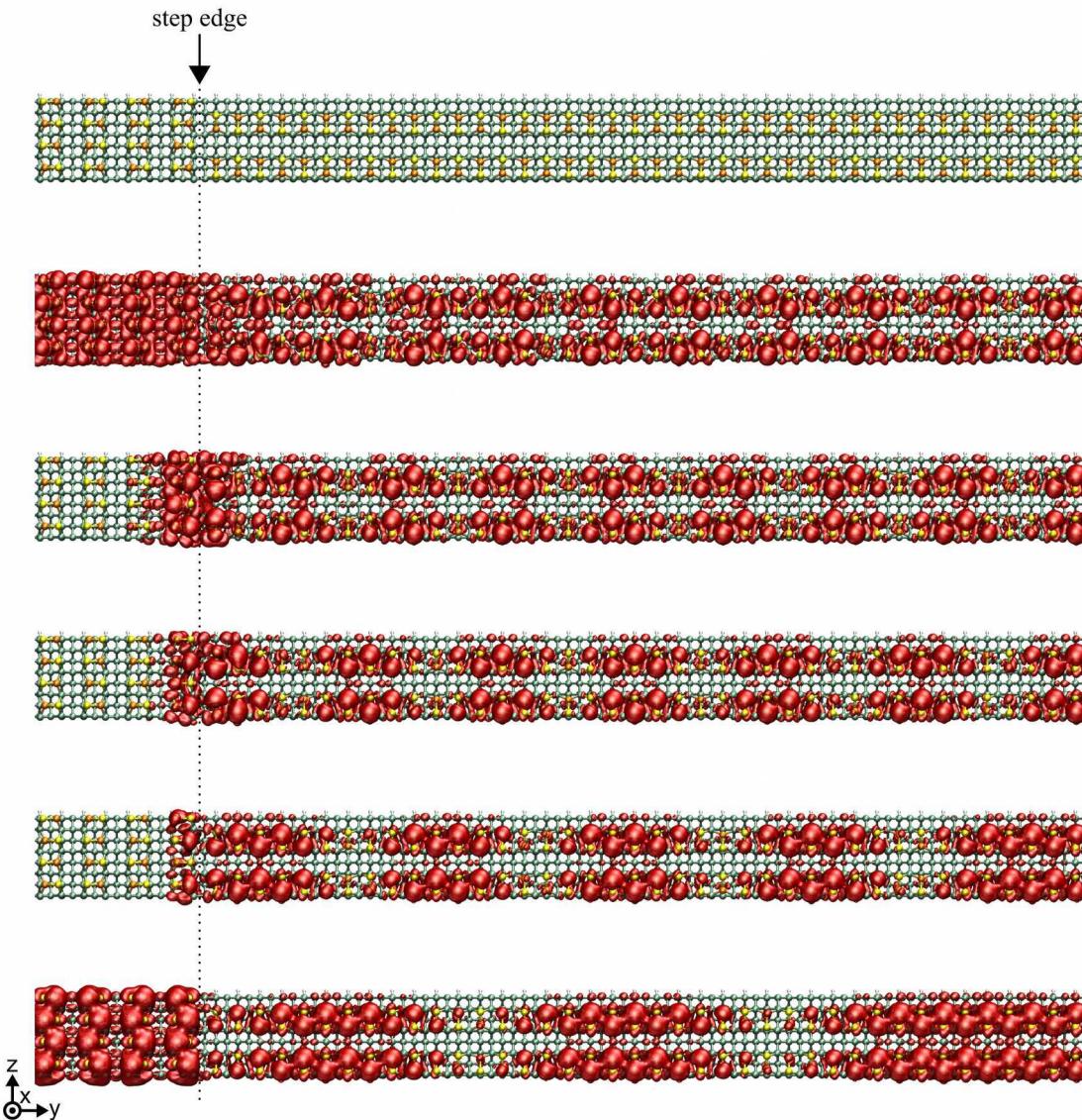
Ge(001) step edge: coherence length



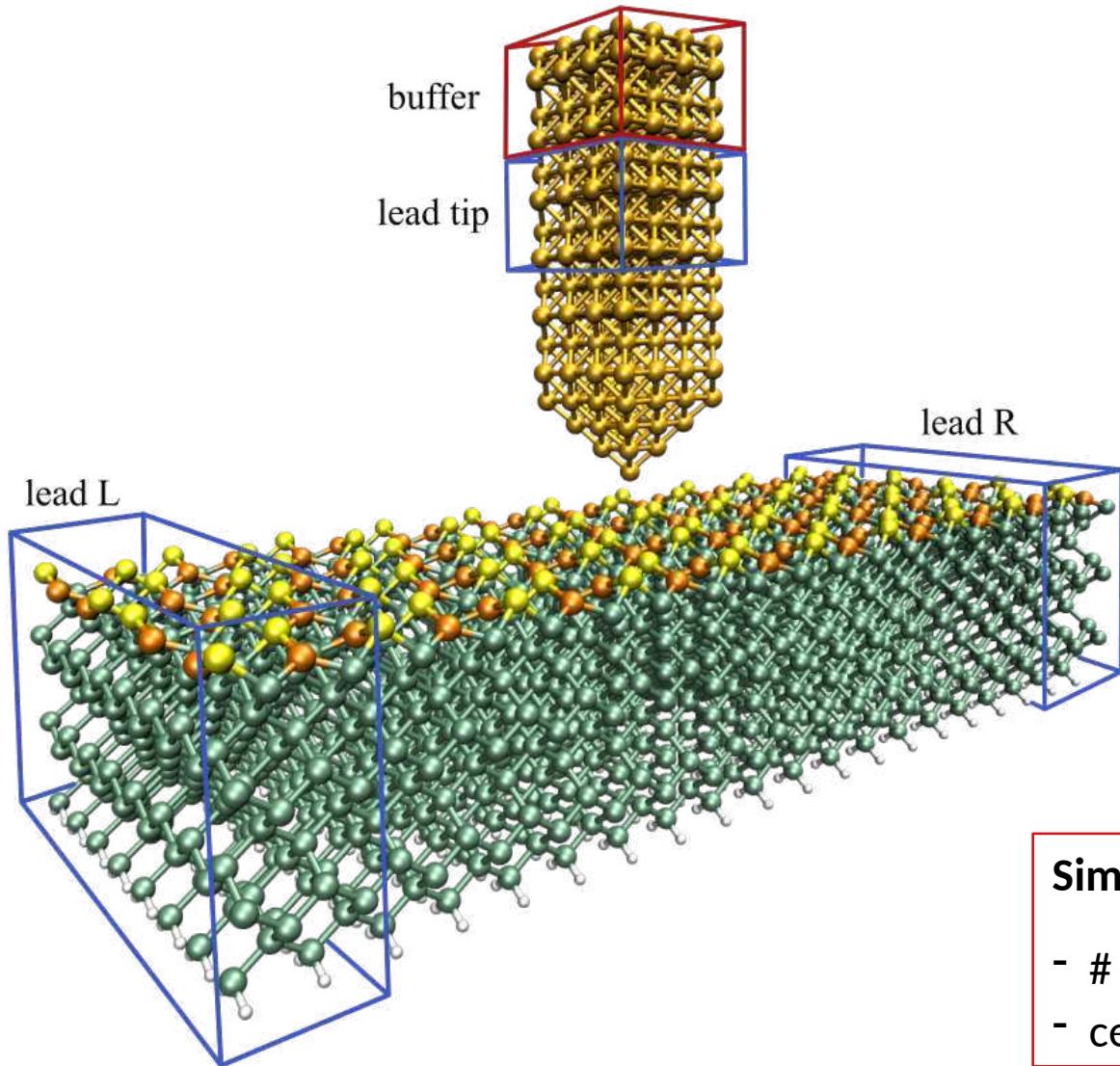
Ge(001) step edge: coherence length



Ge(001) step edge: coherence length



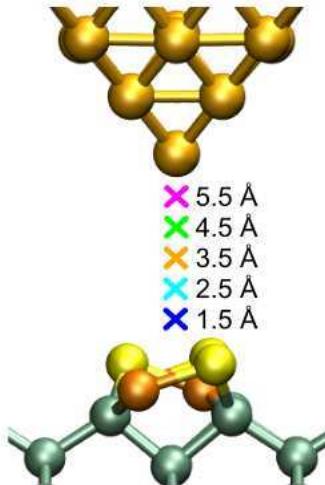
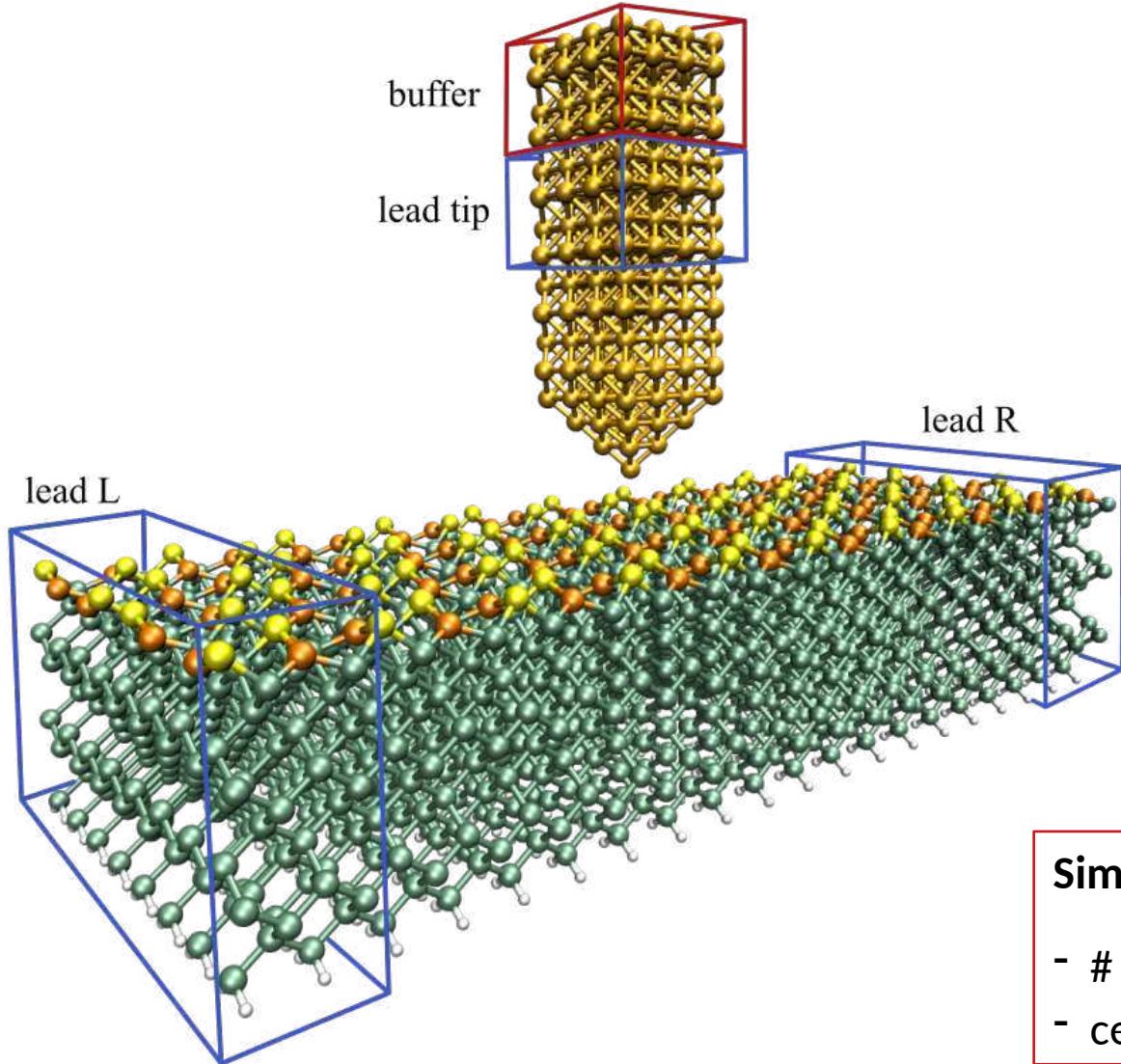
Ge(001) surface addressed by a single tip: 3-terminal setup



Simulation characteristics:

- # of atoms/orbitals: **2462/18221**
- cell size: **32.03x80.07x80 Å³**

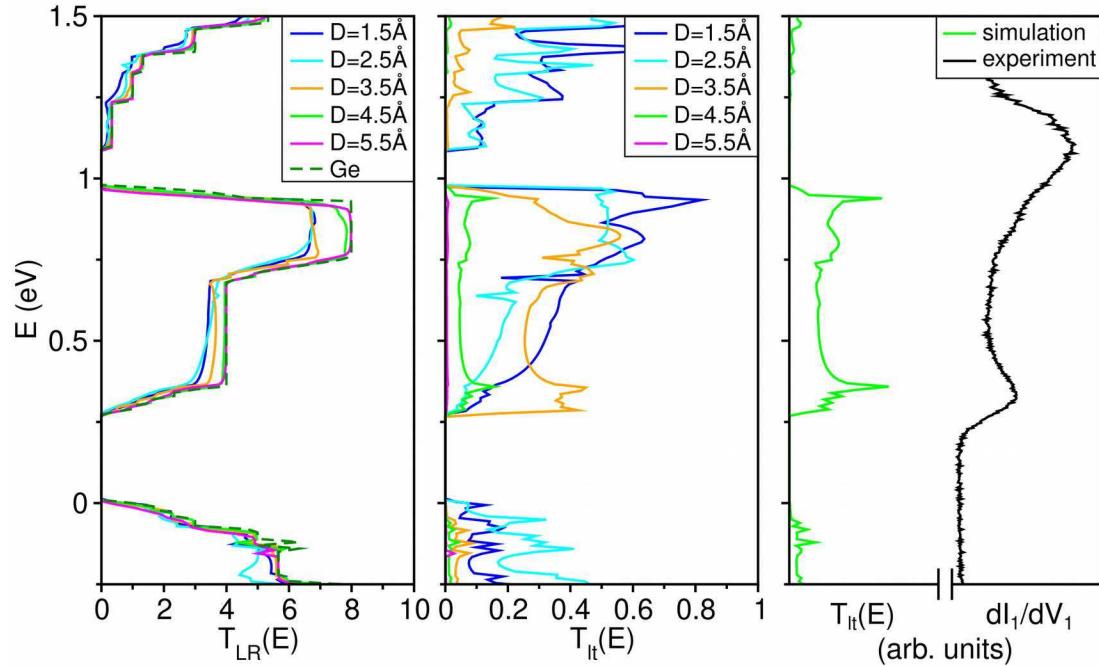
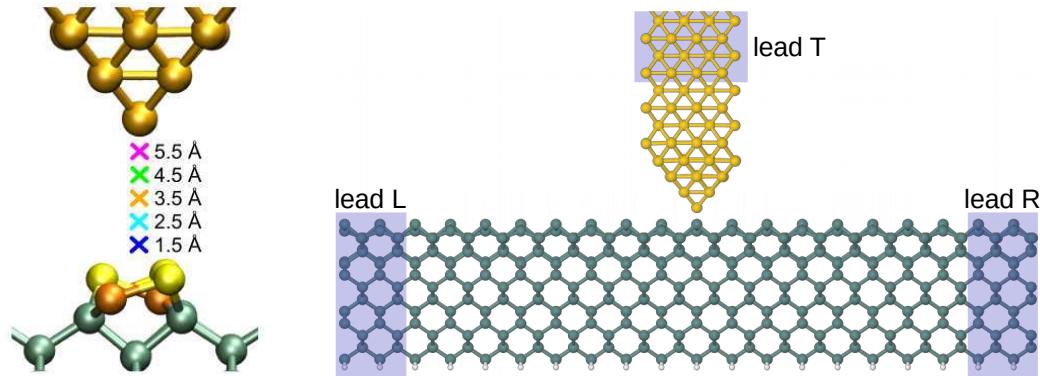
Ge(001) surface addressed by a single tip: 3-terminal setup



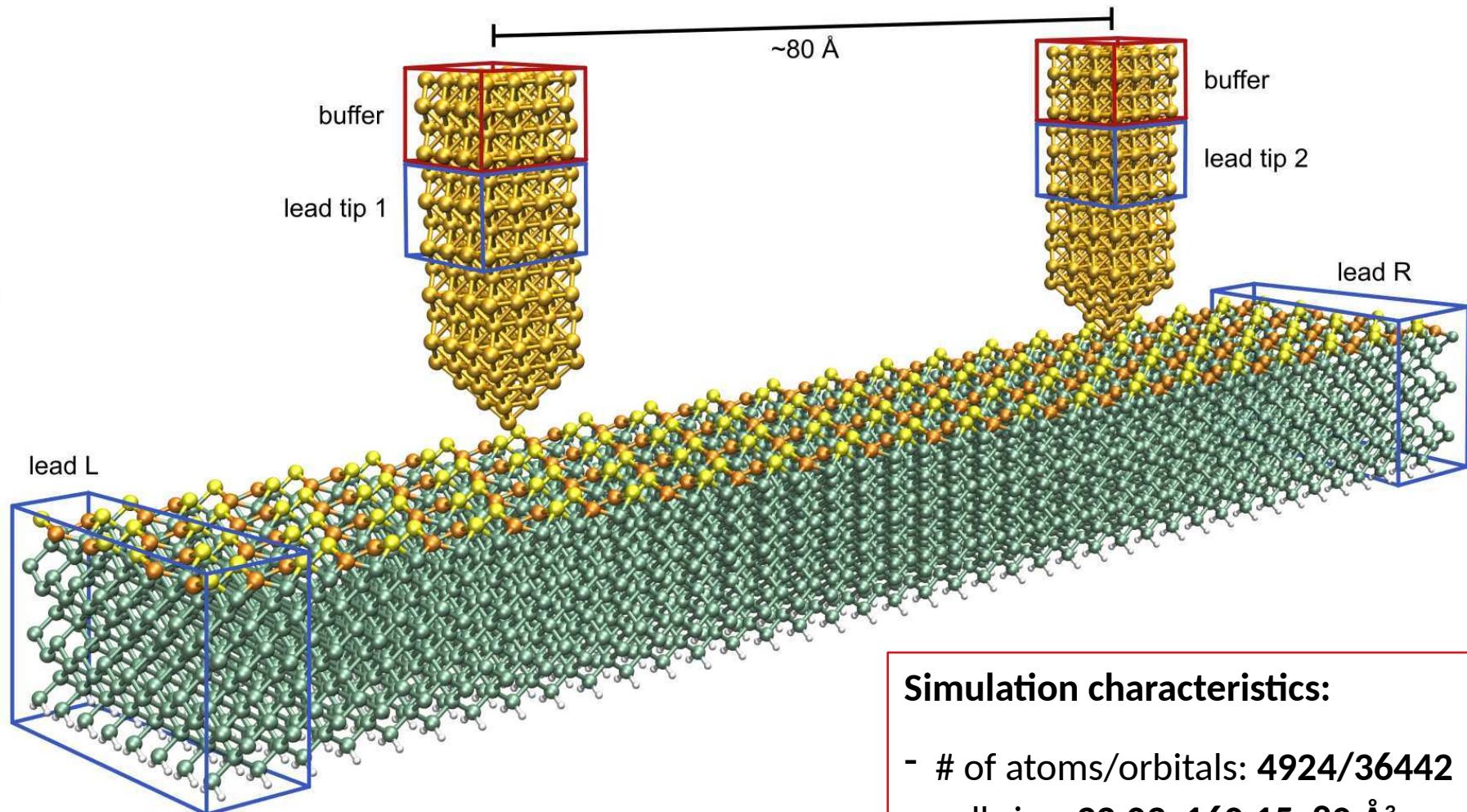
Simulation characteristics:

- # of atoms/orbitals: **2462/18221**
- cell size: **32.03x80.07x80 Å³**

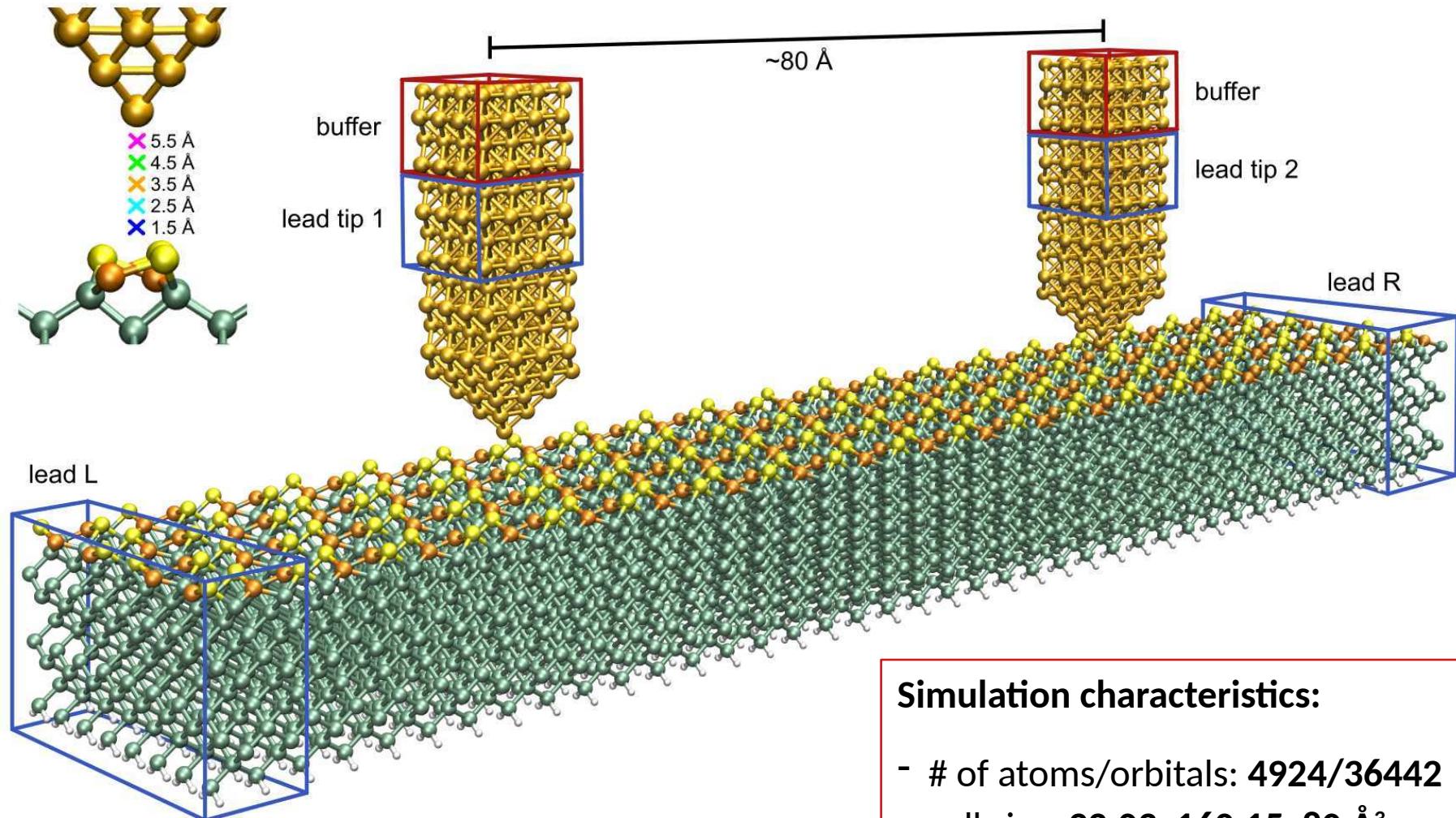
Ge(001) surface addressed by a single tip: 3-terminal setup



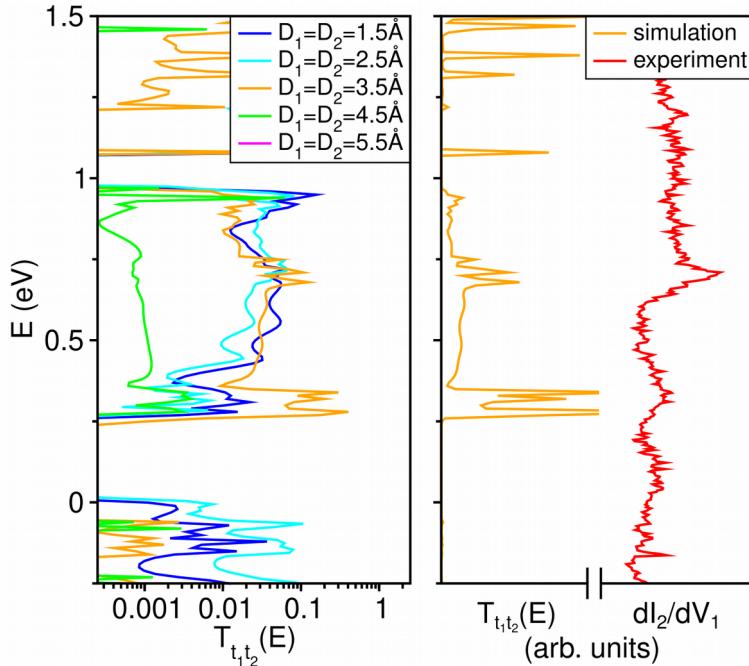
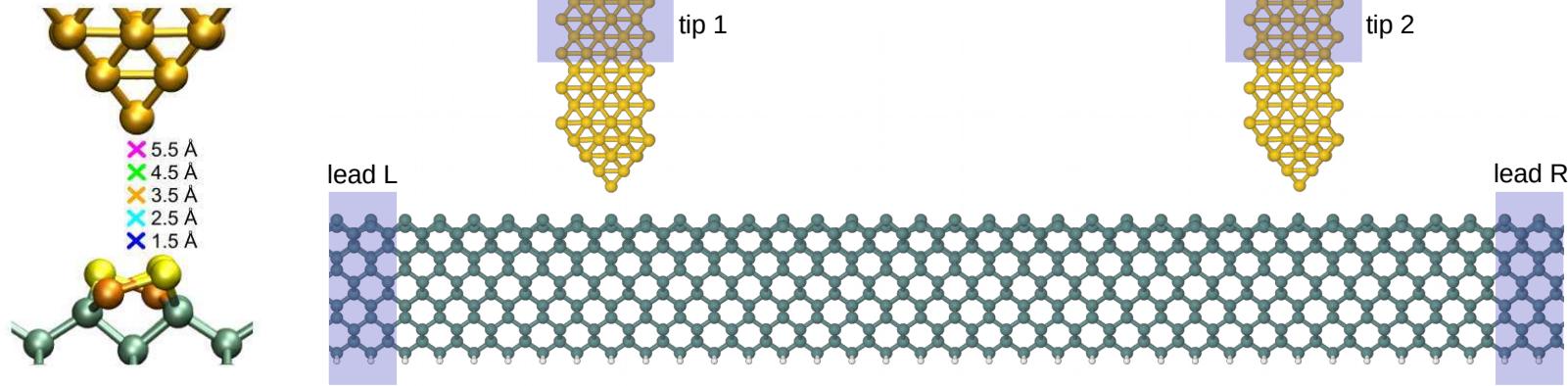
Ge(001) surface addressed by two tips: 4-terminal setup



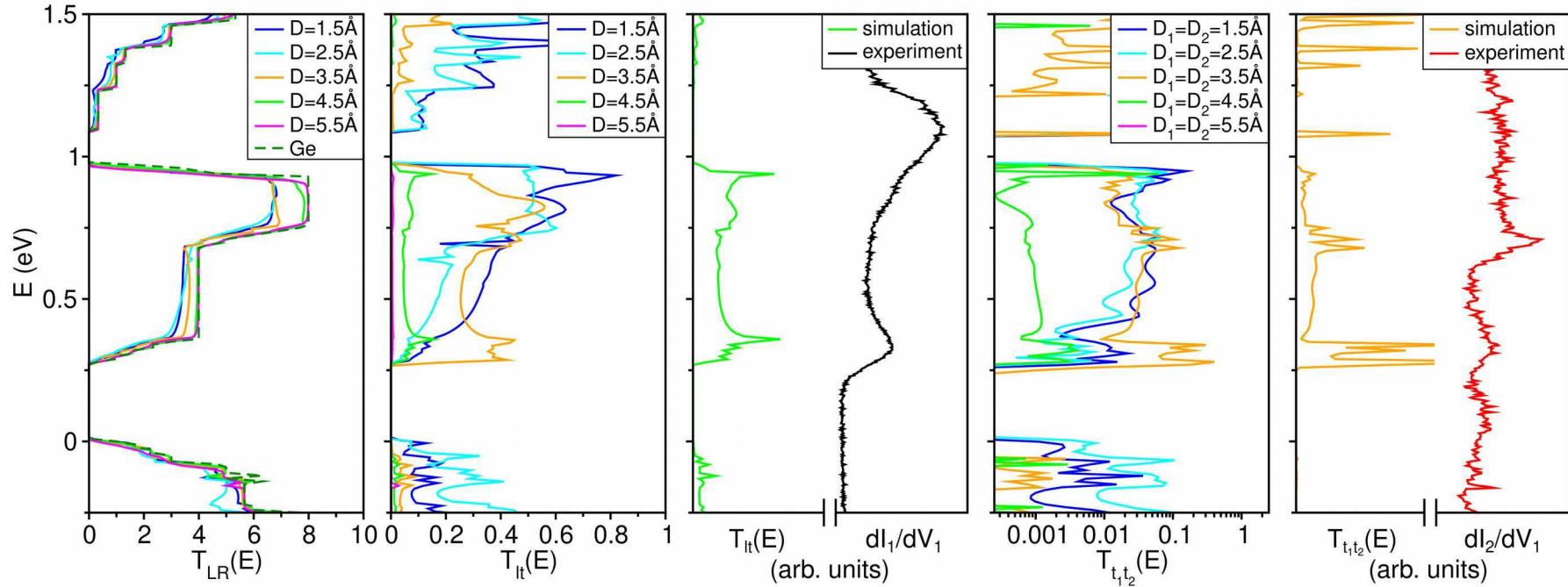
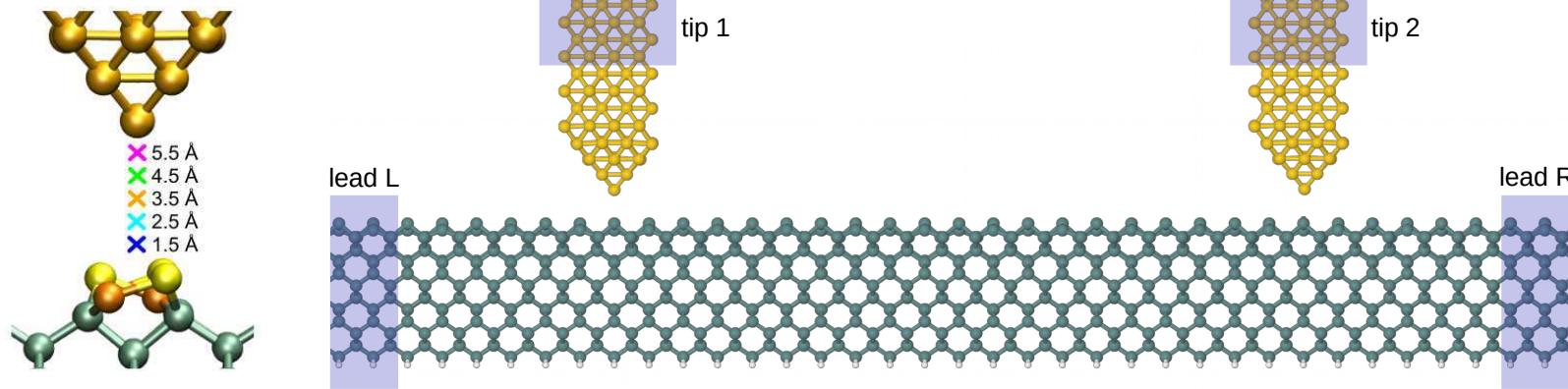
Ge(001) surface addressed by two tips: 4-terminal setup



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



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



Conclusions

- Identification and characterization of the **quasi 1D transport** surface channels **along a single dimer row** on bare Ge(001)-c(4×2) surface;
- SP-STM/STS and calculated eigenchannels on a step-edge confirms a **coherent transport length up to 50nm**;
- TP-STS **planar transconductance** resonances measured with a tip-to-tip distance down to **30nm** and **confirmed by multi-terminal DFT-NEGF simulations**.



Thank you!



MINISTERIO
DE ECONOMÍA
Y COMPETITIVIDAD



CSIC
CONSEJO SUPERIOR DE INVESTIGACIONES CIENTÍFICAS