



Quasi-ballistic transport through surface states of Ge(001)-c(4x2) demonstrated by two-probe STM measurements and multi-terminal fist-principles simulations

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

March 13, 2018



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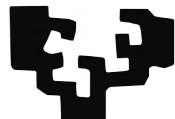
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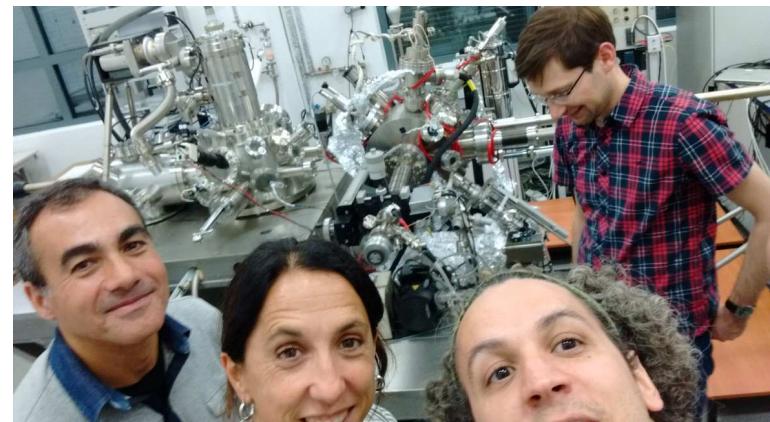
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Two-probe STM at the atomic level



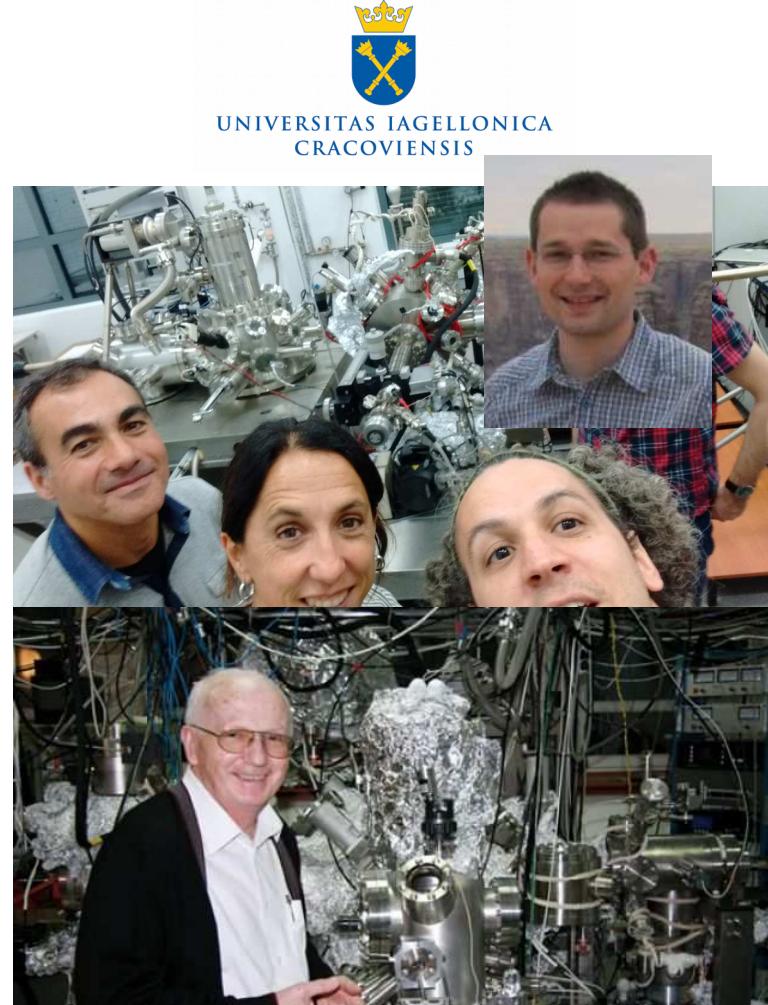


Two-probe STM at the atomic level





Two-probe STM at the atomic level



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

Methods

Density-Functional Theory (DFT)

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)

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Non-Equilibrium Green's Function (NEGF)

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

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Multi-terminal!!!

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Methods

General parameters:

- pseudo: **ca** for Ge and H,
car for Au
- functional: **Ida-ca**
- basis: **DZ** for Ge and H,
s-DZP/d-SZ for Au,
diffusive s-orbital at apex Au
- energy shift: **100 meV**
- real space grid cutoff: **250 Ry**
- k-grid: **3X1X1**
- elect. Temp. 300 K
- DM tol. < 1.d-5
- H tol. < 1.d-4 eV

Density-Functional Theory (DFT)

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Non-Equilibrium Green's Function (NEGF)

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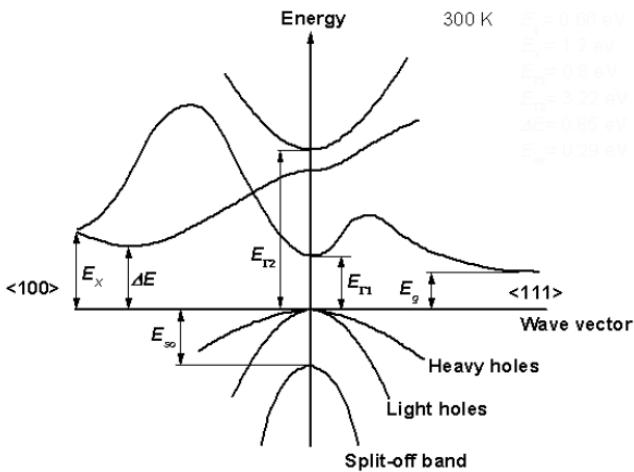
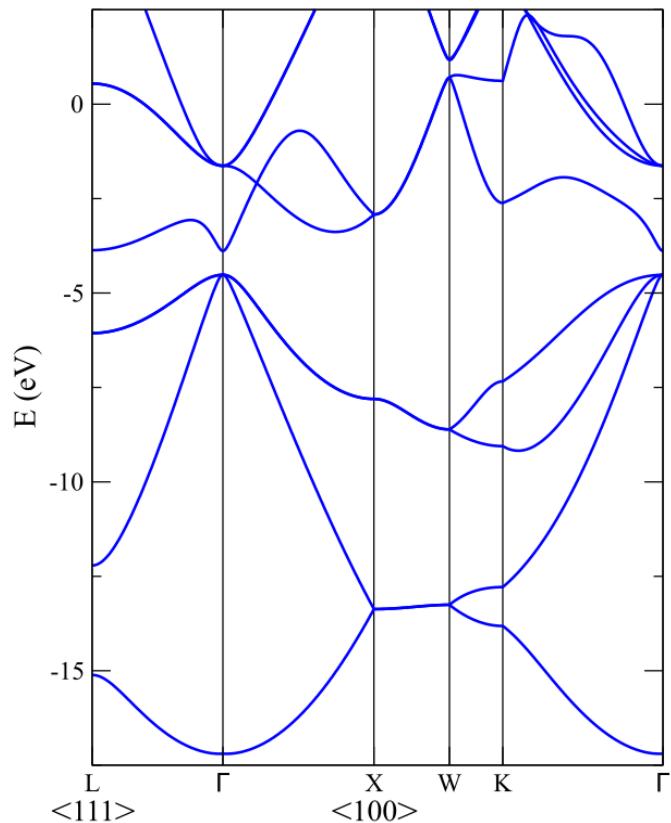
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Methods

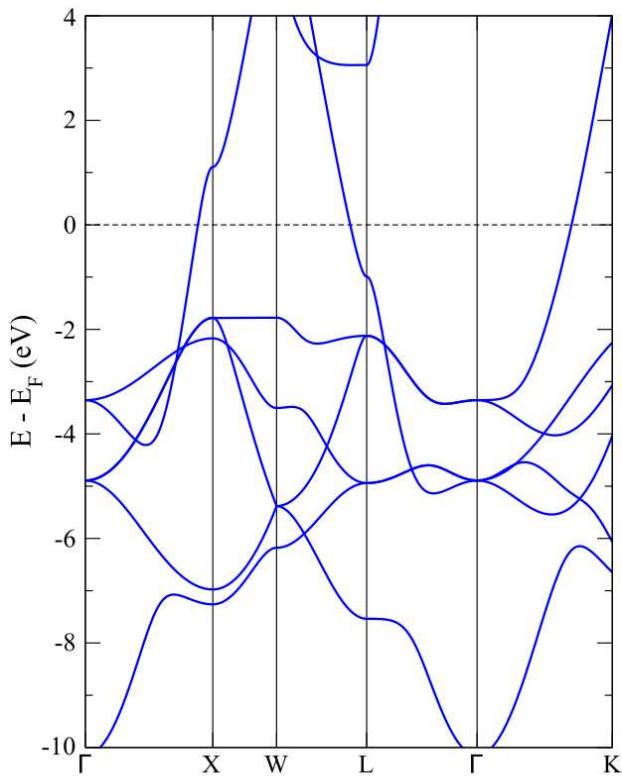


	Exp*	ca-DZP	ca-DZ	car-DZP
$a(\text{\AA})$	5.660	5.638	5.662	5.656
$E_g(\text{eV})$	0.661	0.566	0.632	0.098
$E_X(\text{eV})$	1.2	0.809	1.596	0.679
$E_{r1}(\text{eV})$	0.8	0.951	0.632	0.098
$E_{r2}(\text{eV})$	3.22	2.577	2.886	2.558
$\Delta E(\text{eV})$	0.85	0.615	1.134	0.491

Ge parameters:

- T.-M. pseudo: **ca**
- xc functional: **lda-ca**
- basis set size: **DZ**

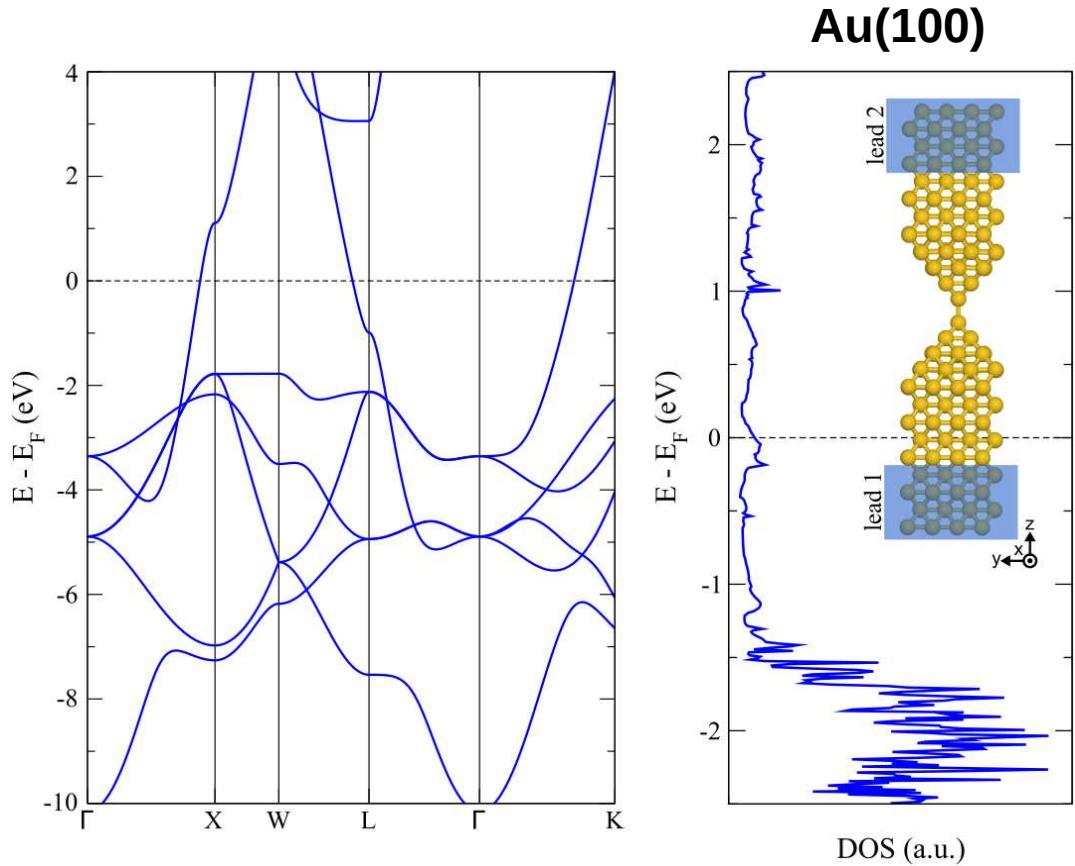
Methods



Au parameters:

- T.-M. pseudo: **car**
- xc functional: **lda-ca**
- basis set size:
s-DZP/d-SZ
extended s for apex

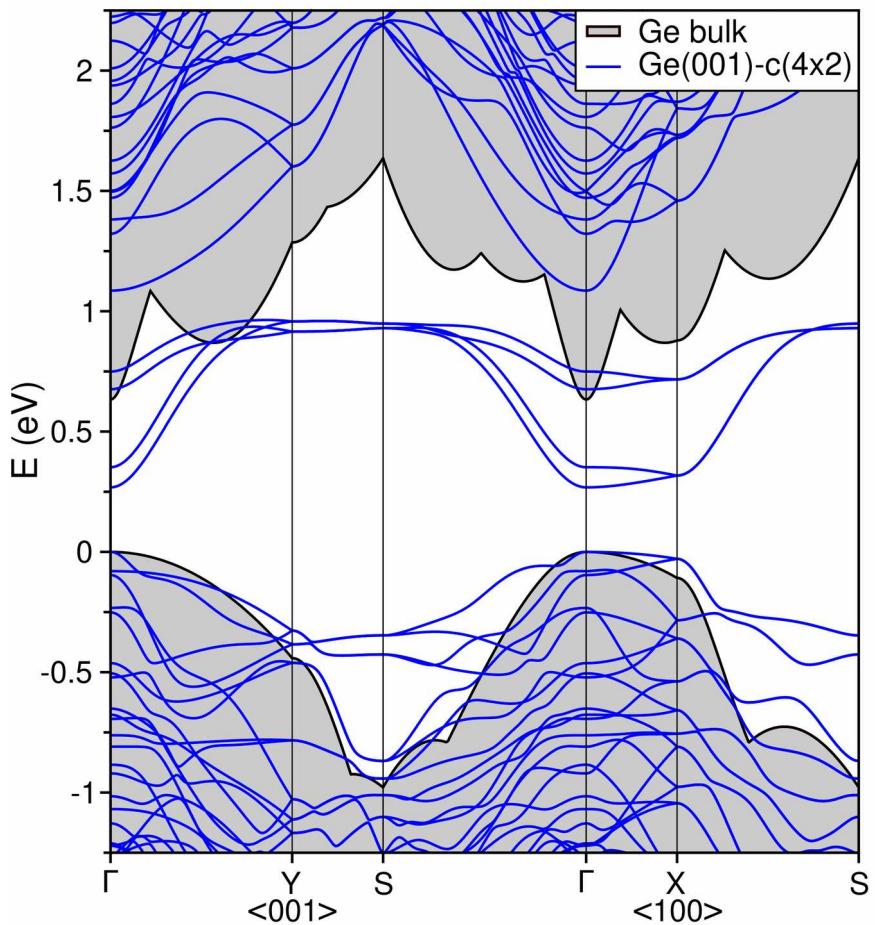
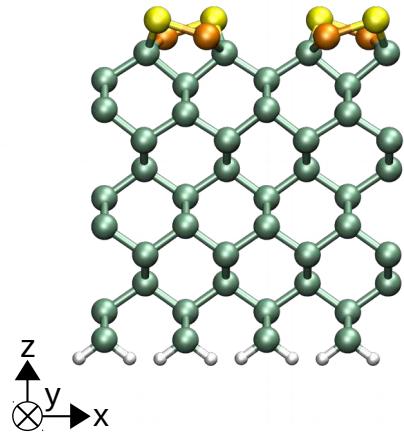
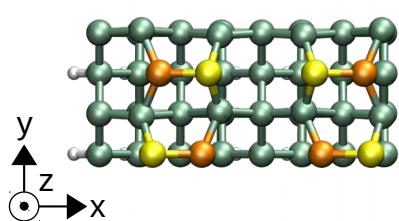
Methods



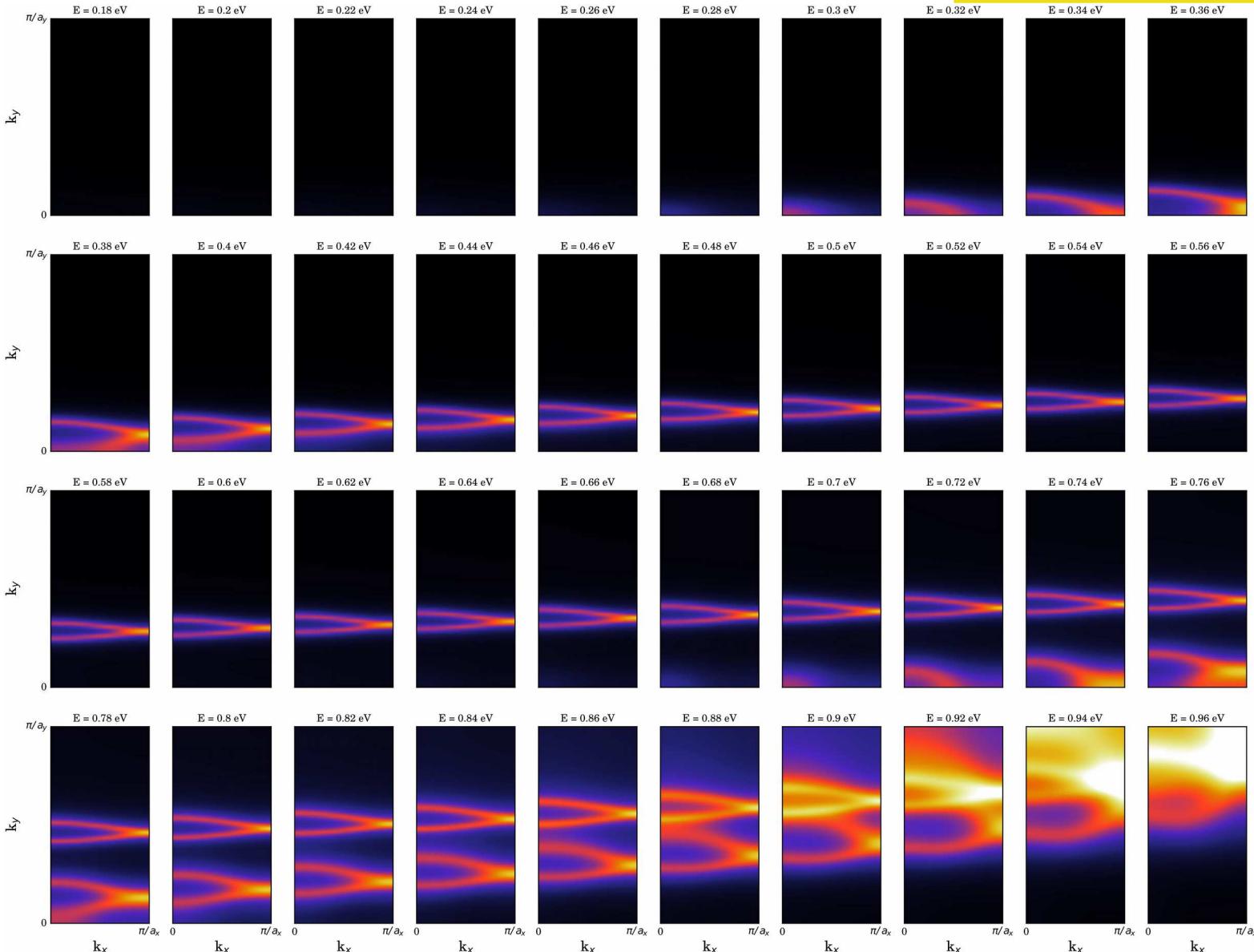
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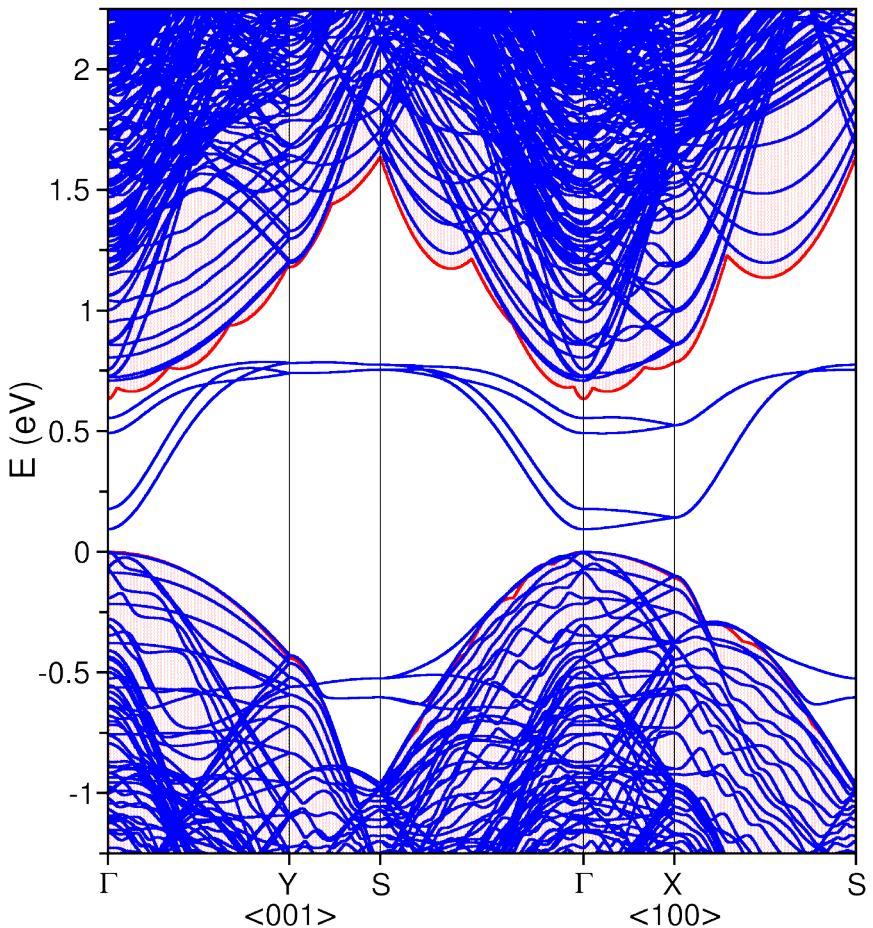
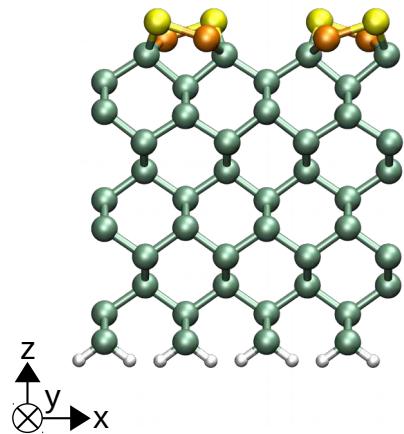
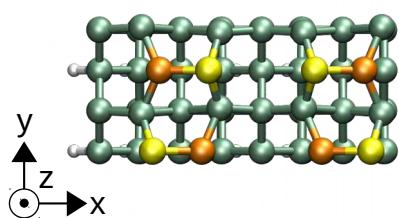
Ge(001)x(4x2) surface



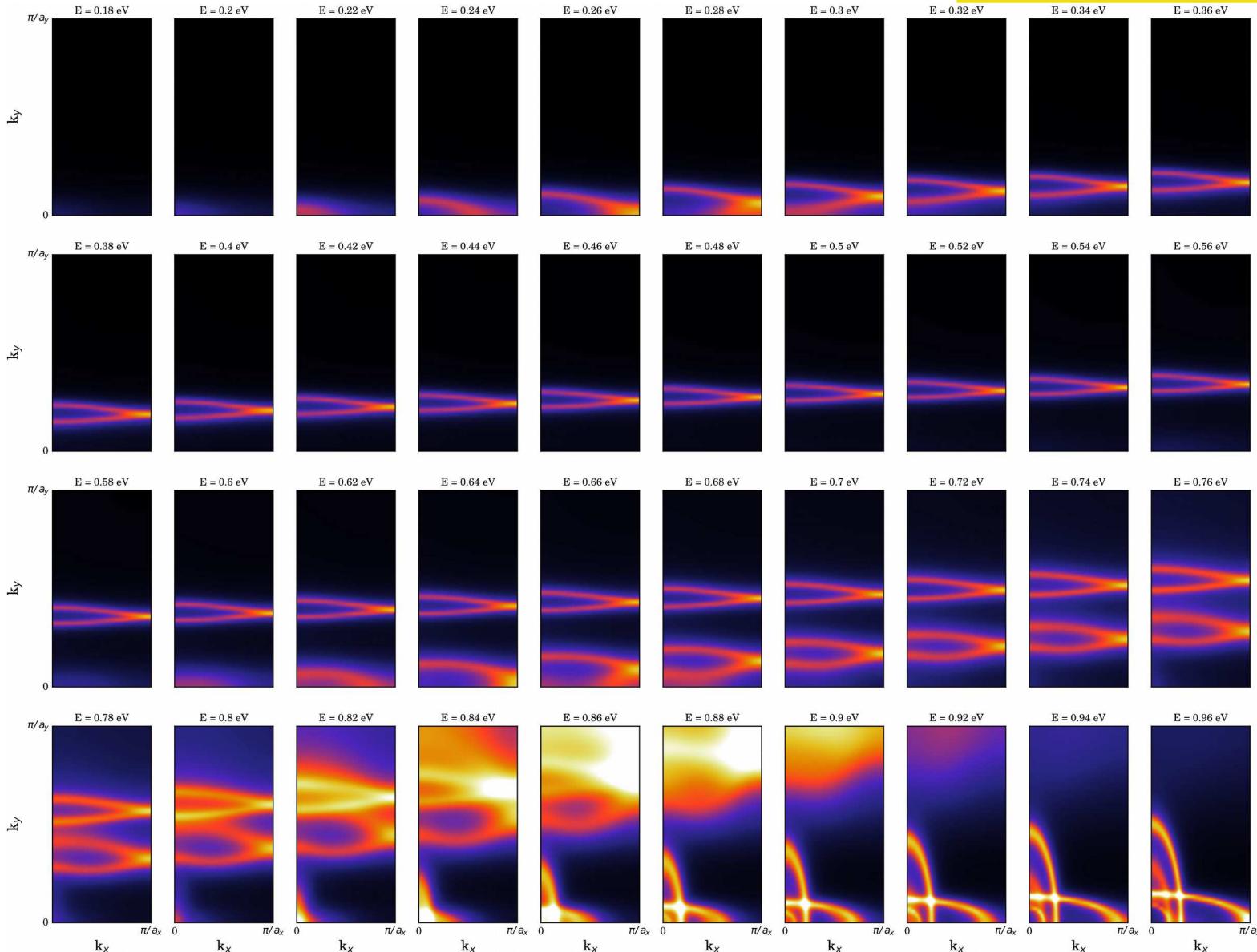
Ge(001)x(4x2) surface



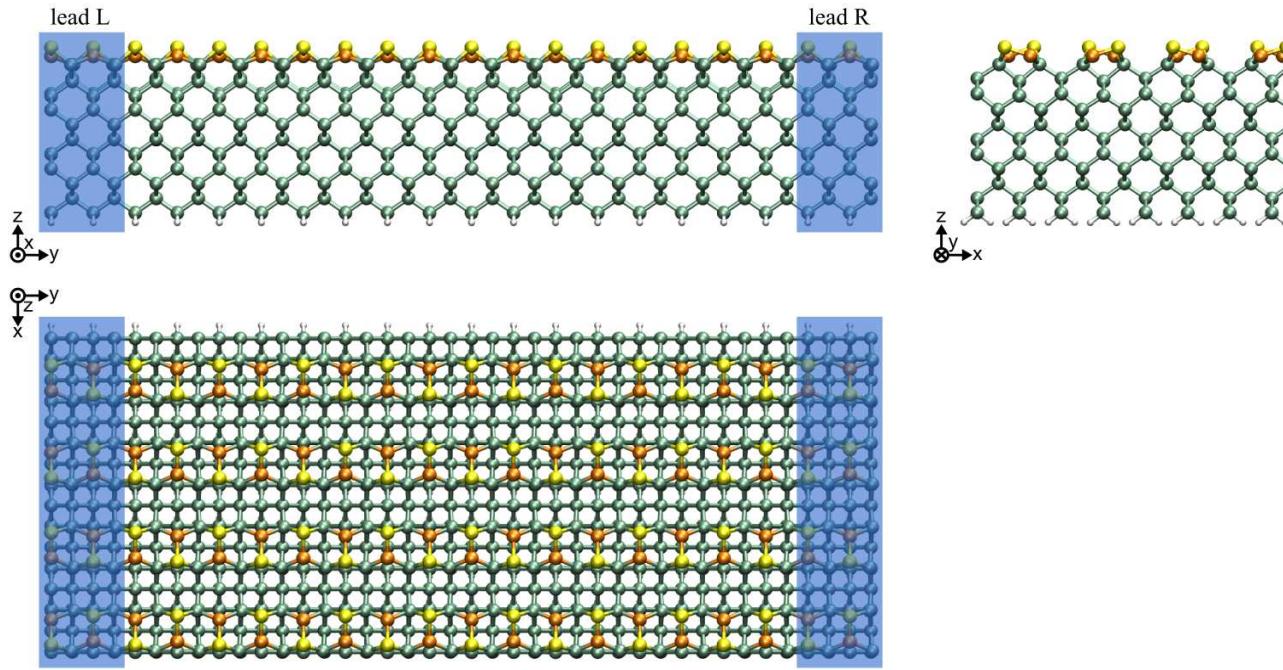
Ge(001)x(4x2) surface



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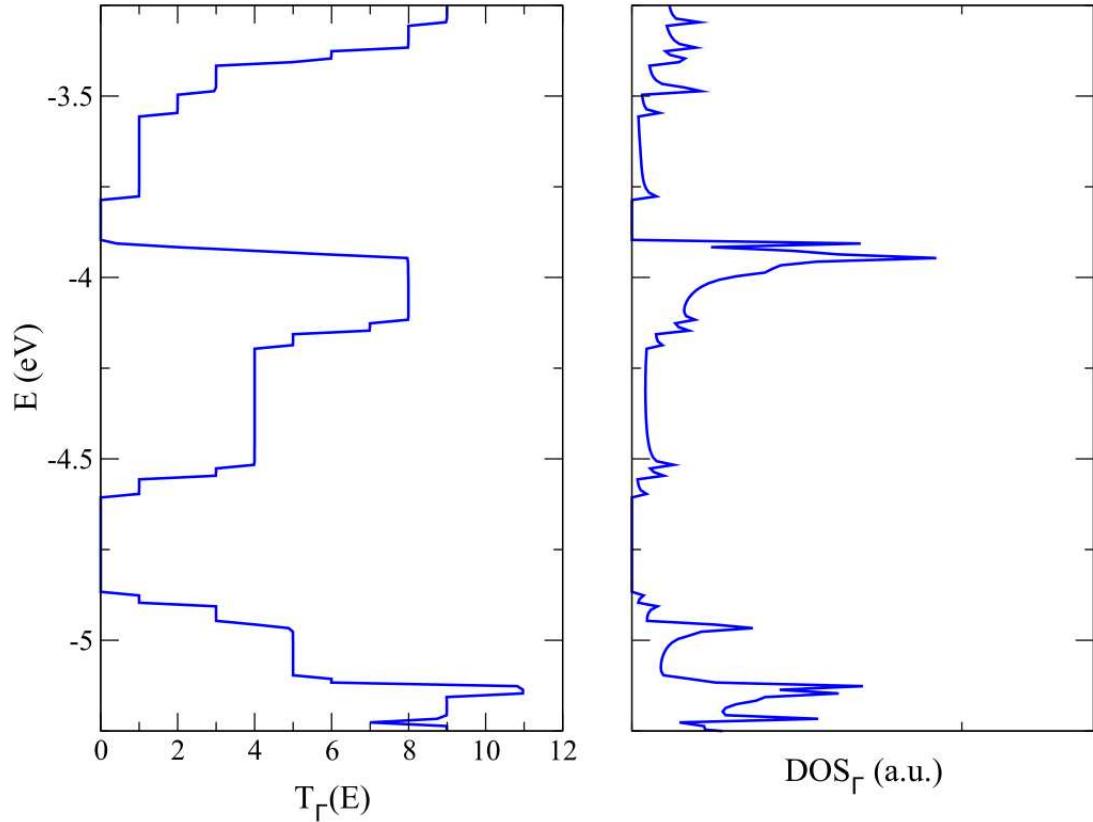
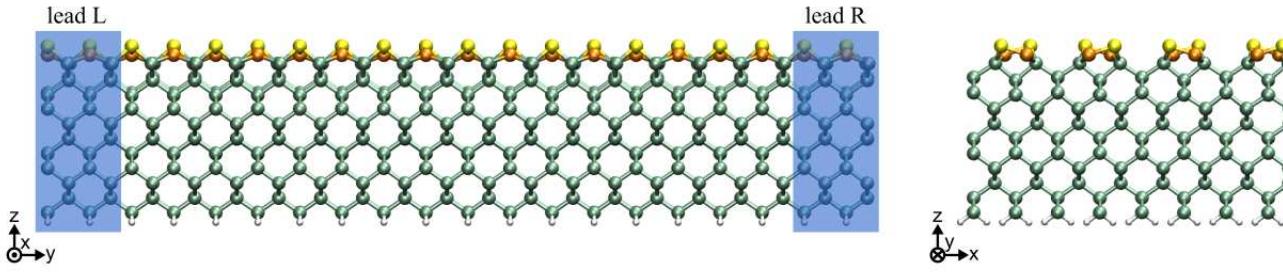
Ge(001) surface: 2-terminal setup



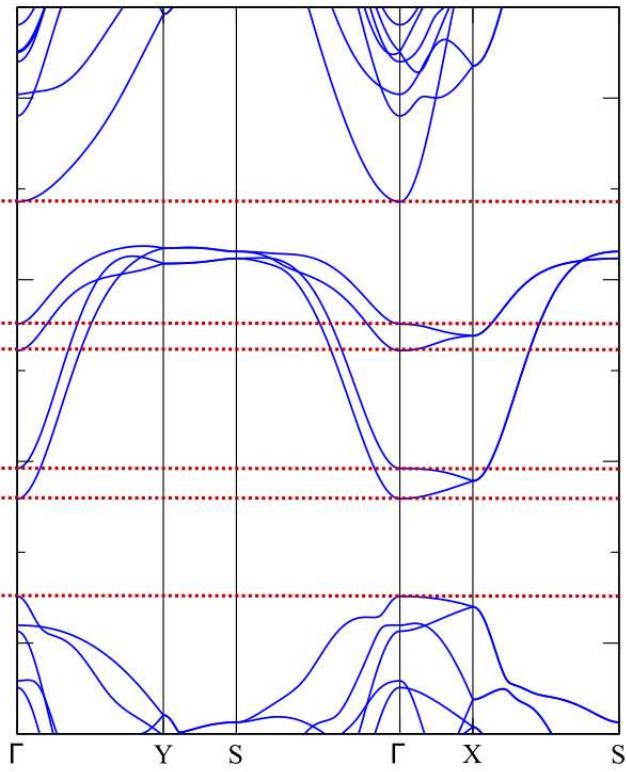
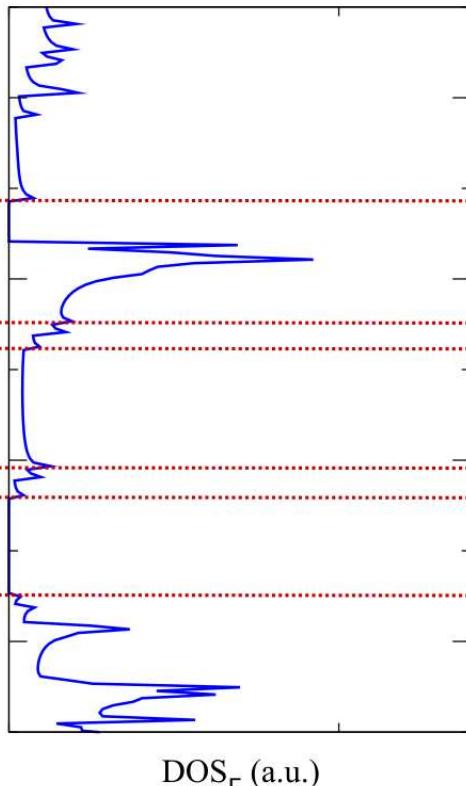
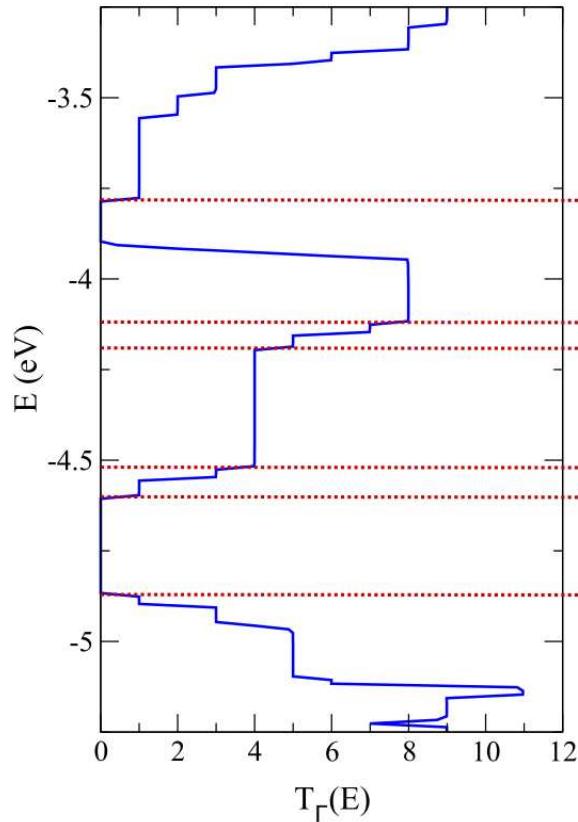
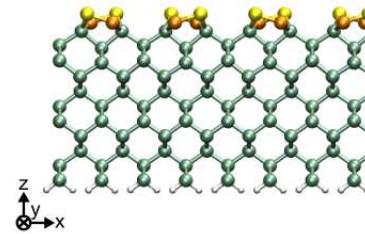
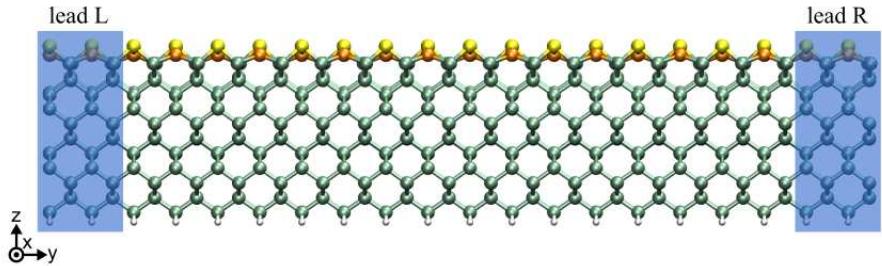
Simulation characteristics:

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

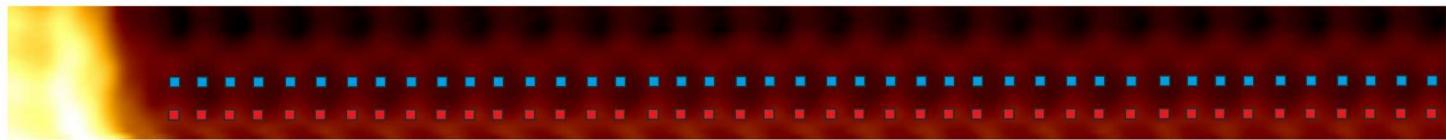
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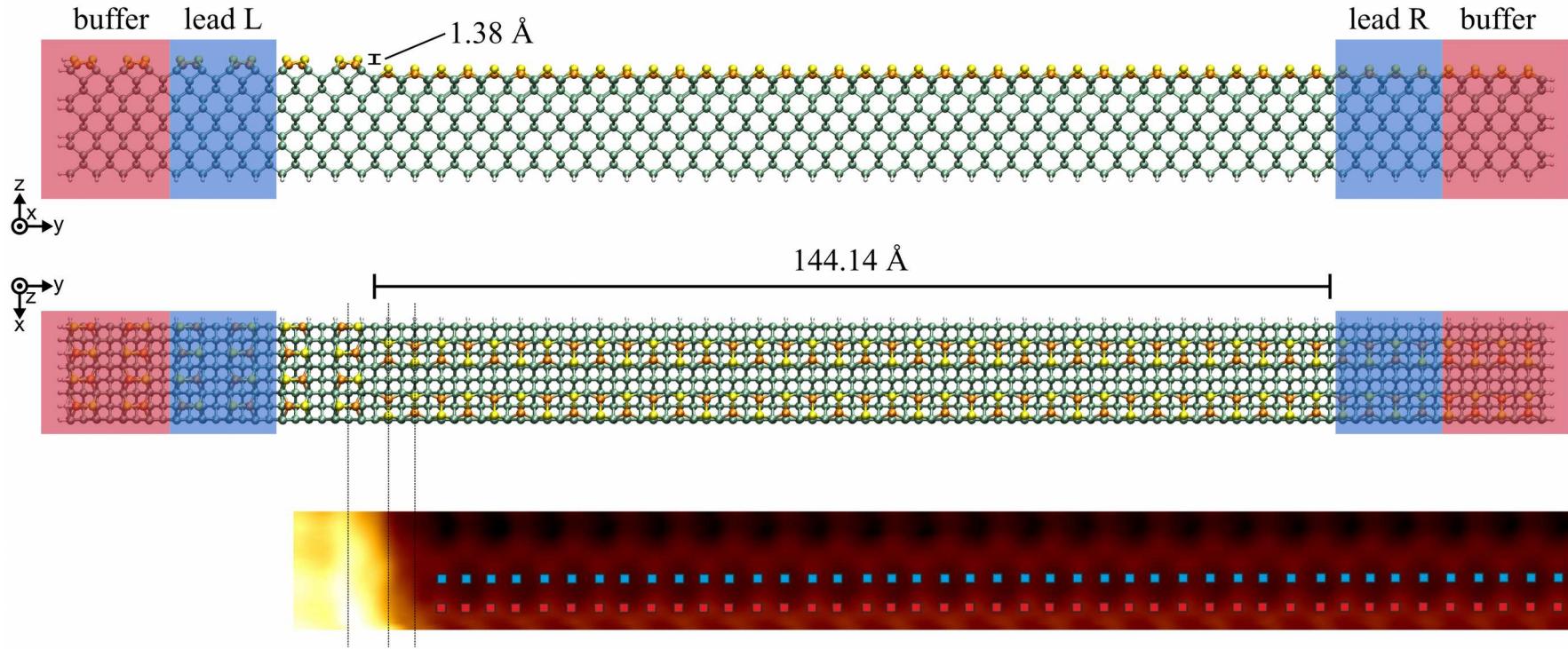
Ge(001) surface: 2-terminal setup



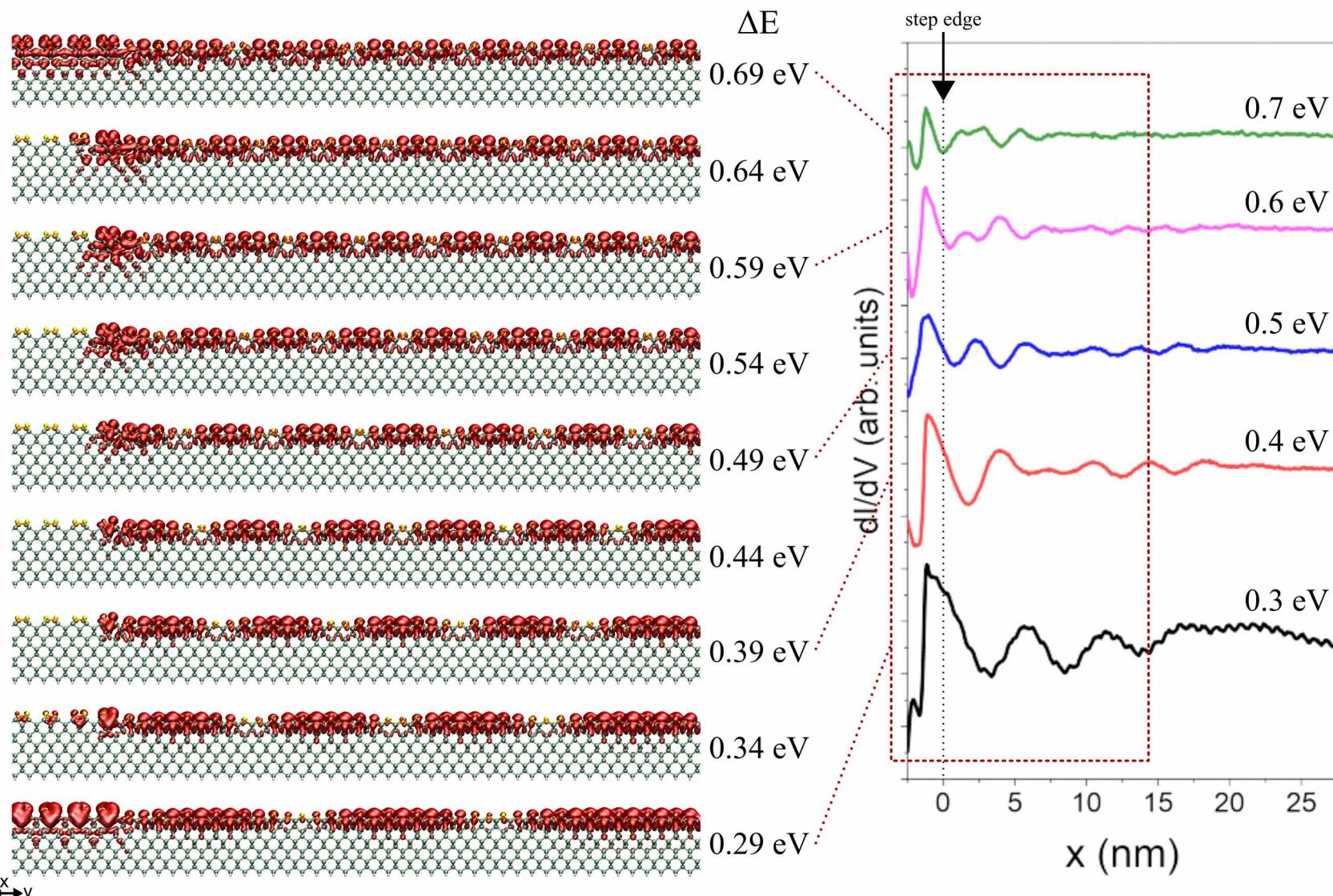
Ge(001) step edge: coherence length



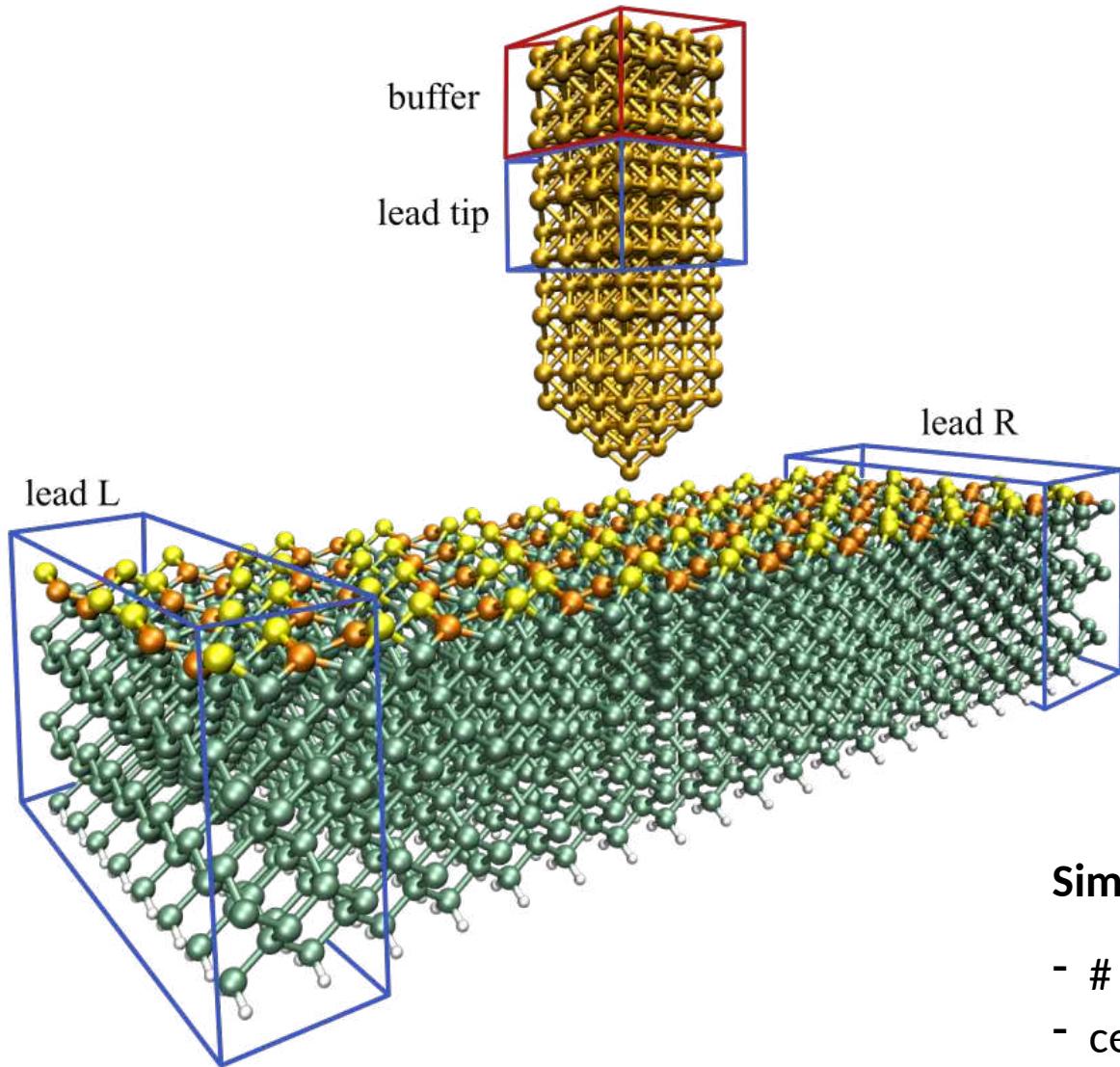
Ge(001) step edge: coherence length



Ge(001) step edge: coherence length



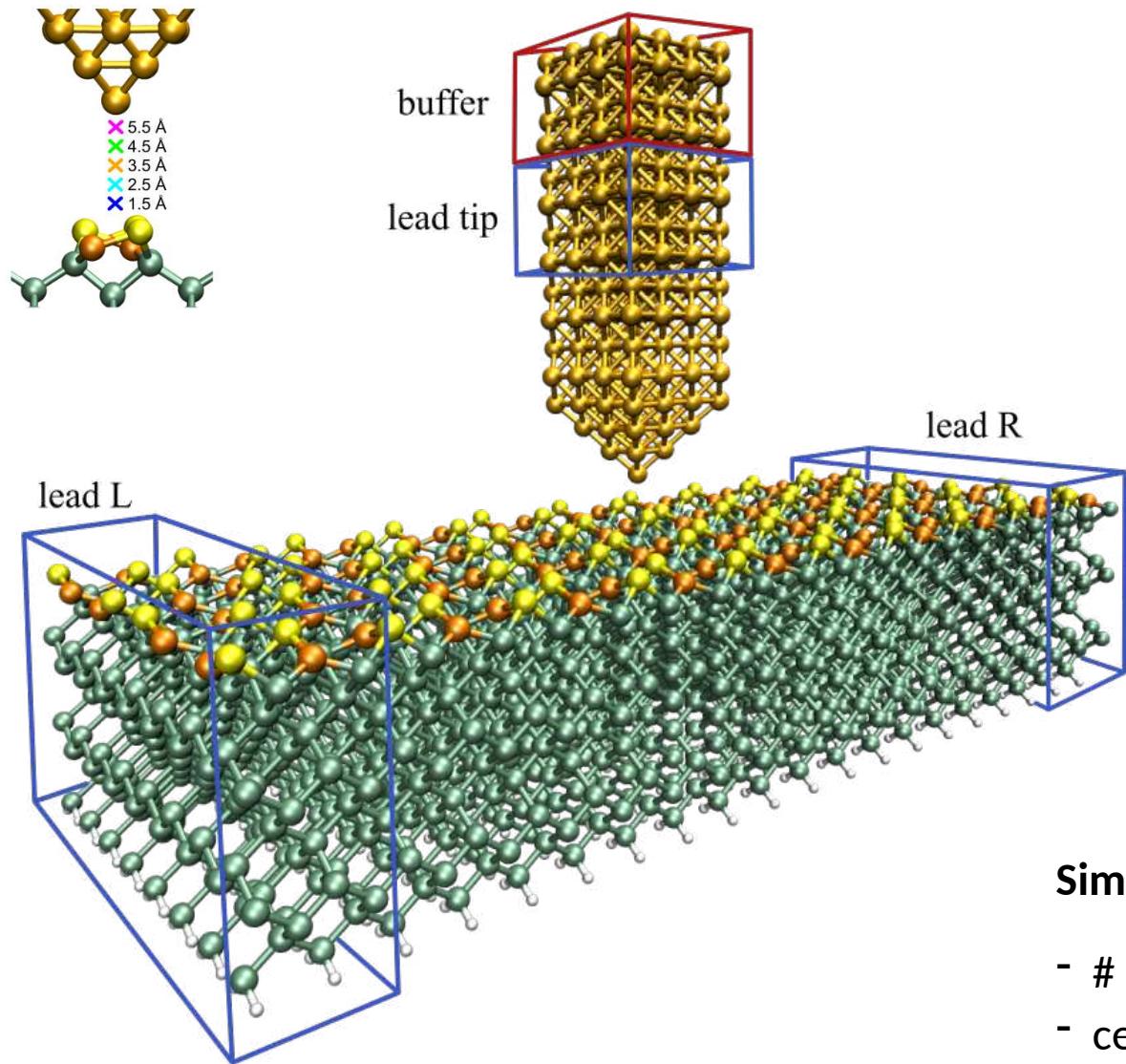
Ge(001) surface addressed by a single tip: 3-terminal setup



Simulation characteristics:

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

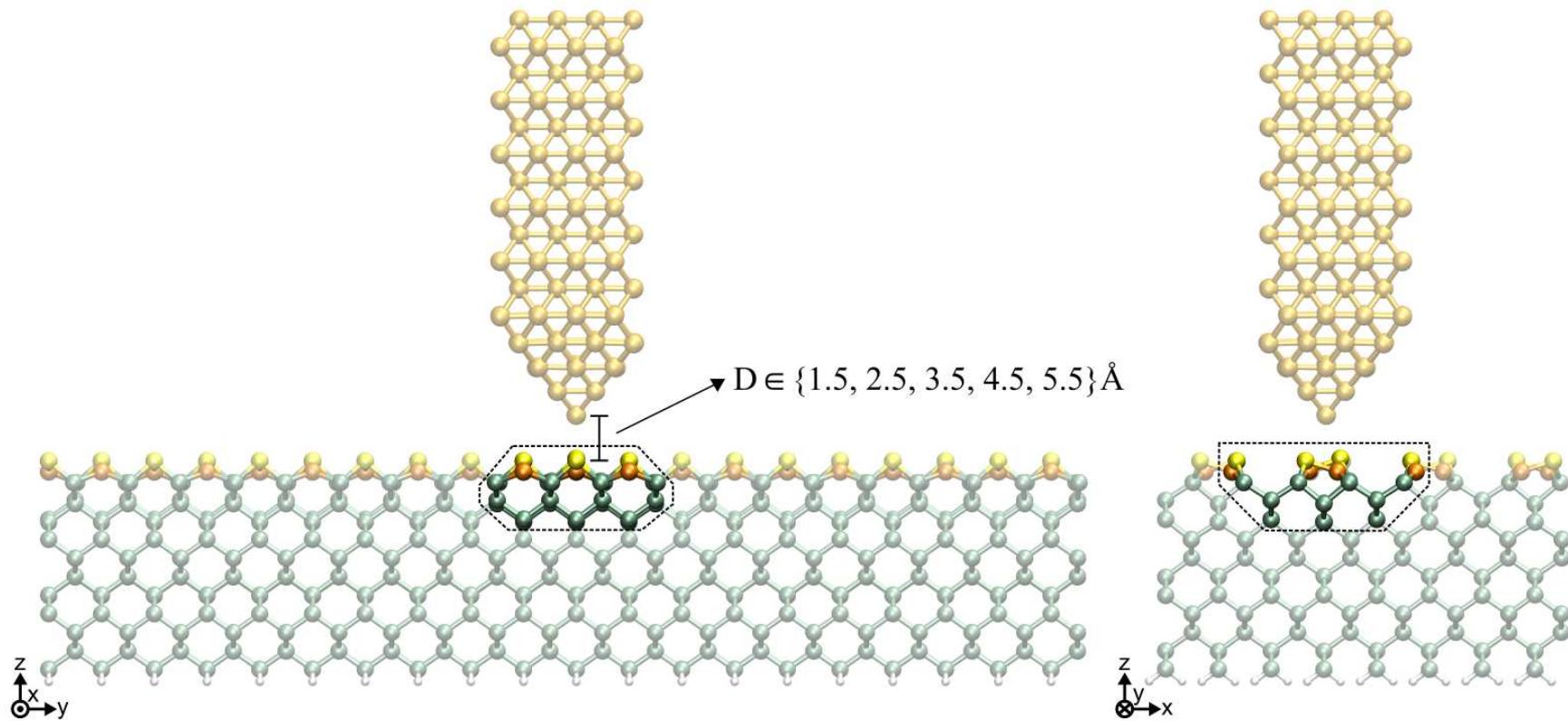
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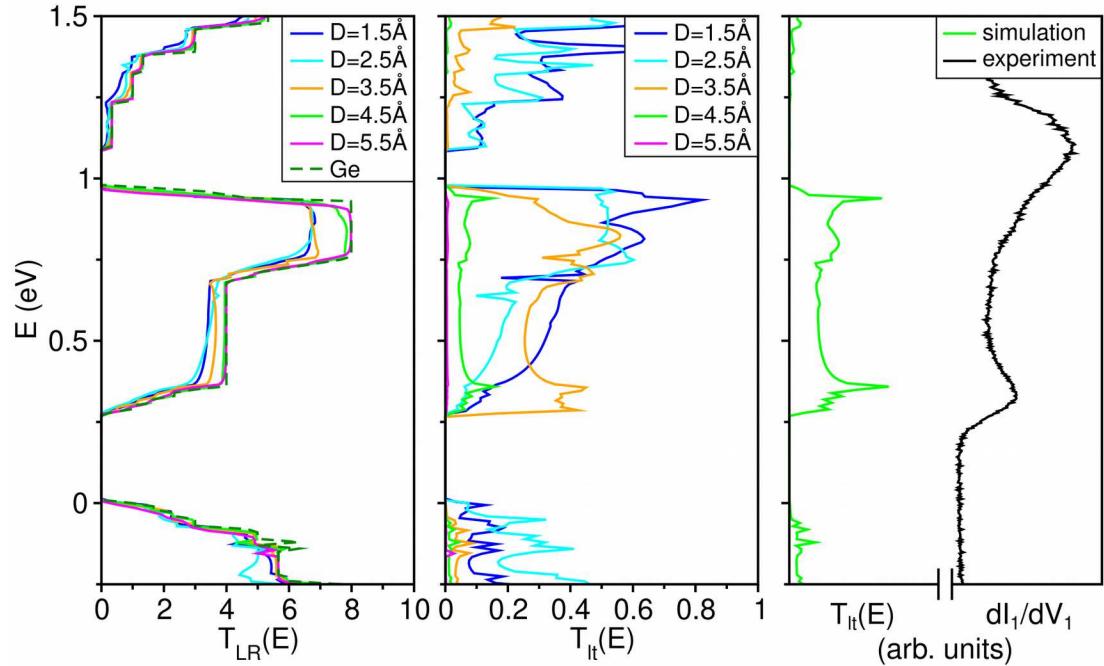
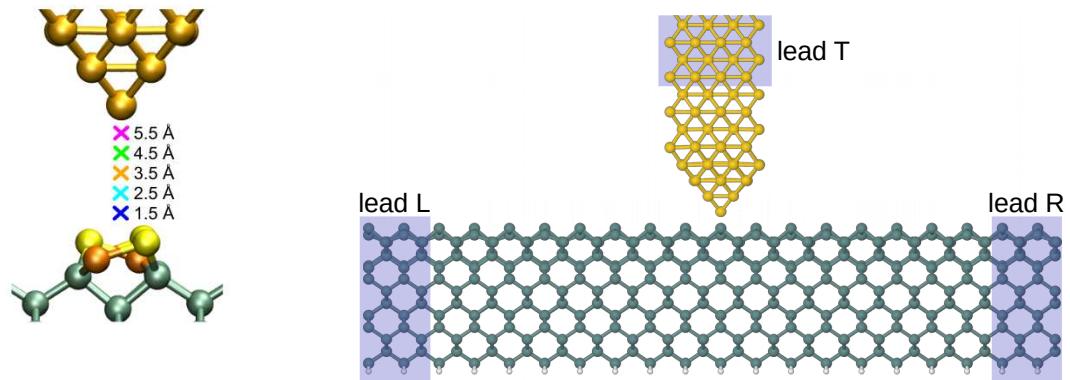
Methods



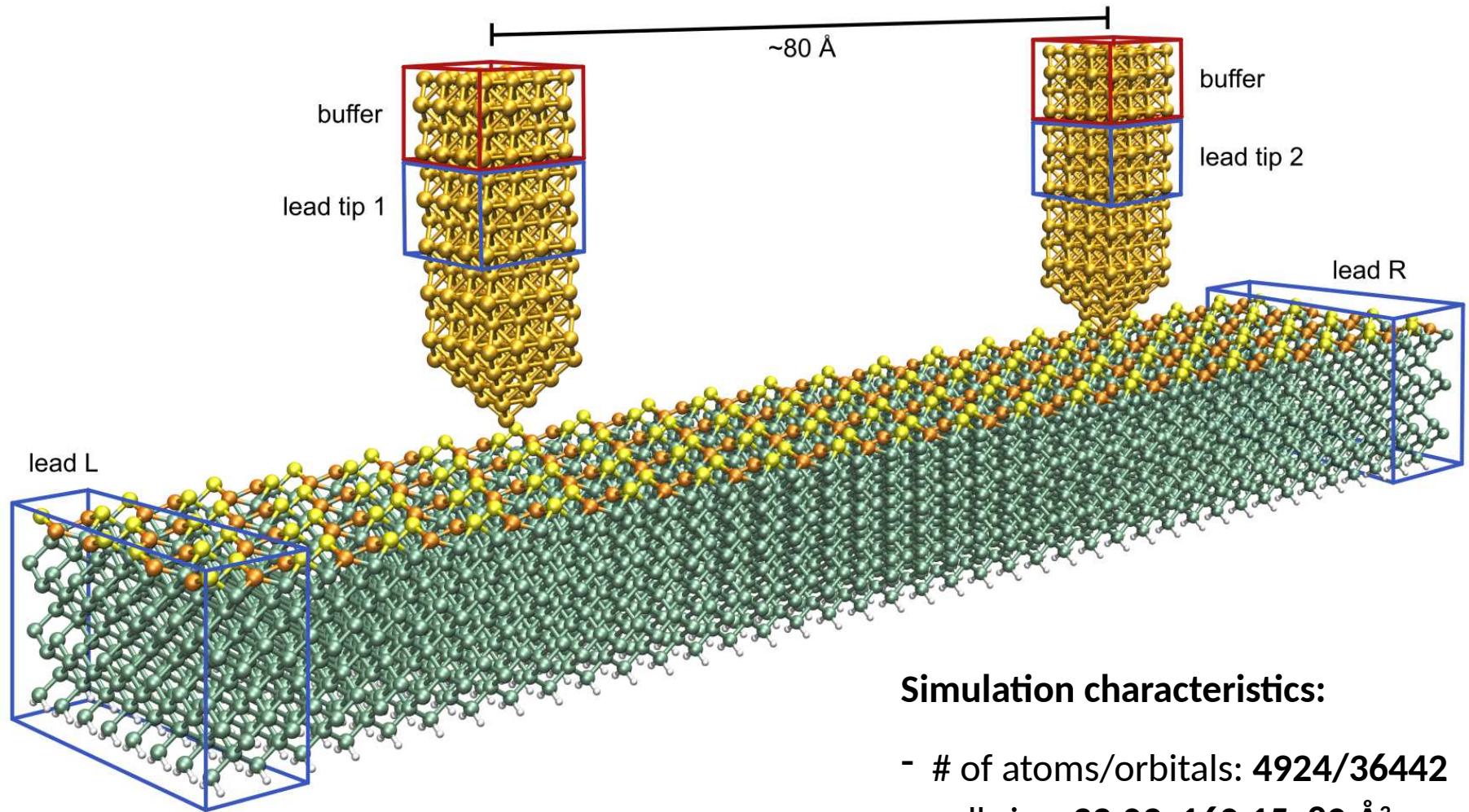
Simulation characteristics:

- # of atoms/orbitals: **2462/18221**
- cell size: **32.03x80.07x80 Å³**
- forces < 0.1 eV/Å

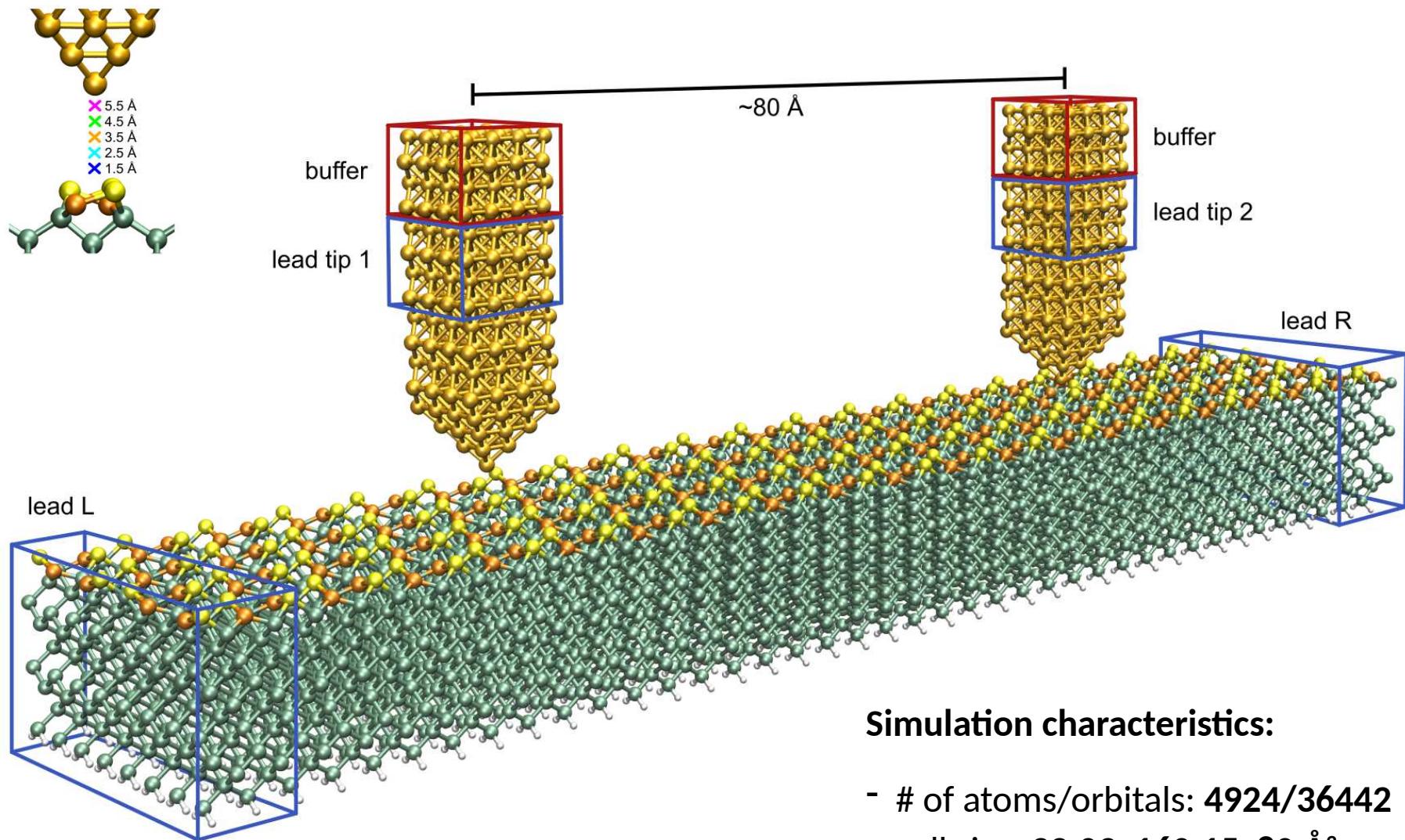
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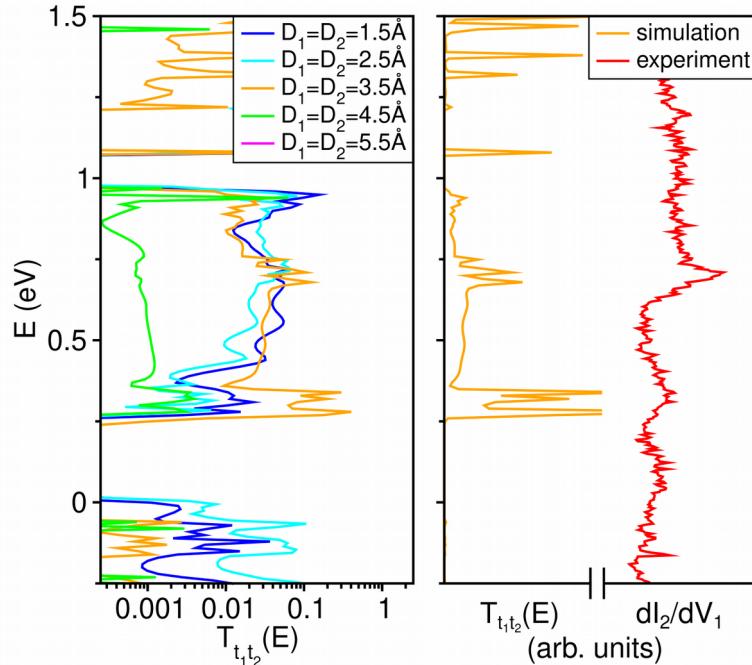
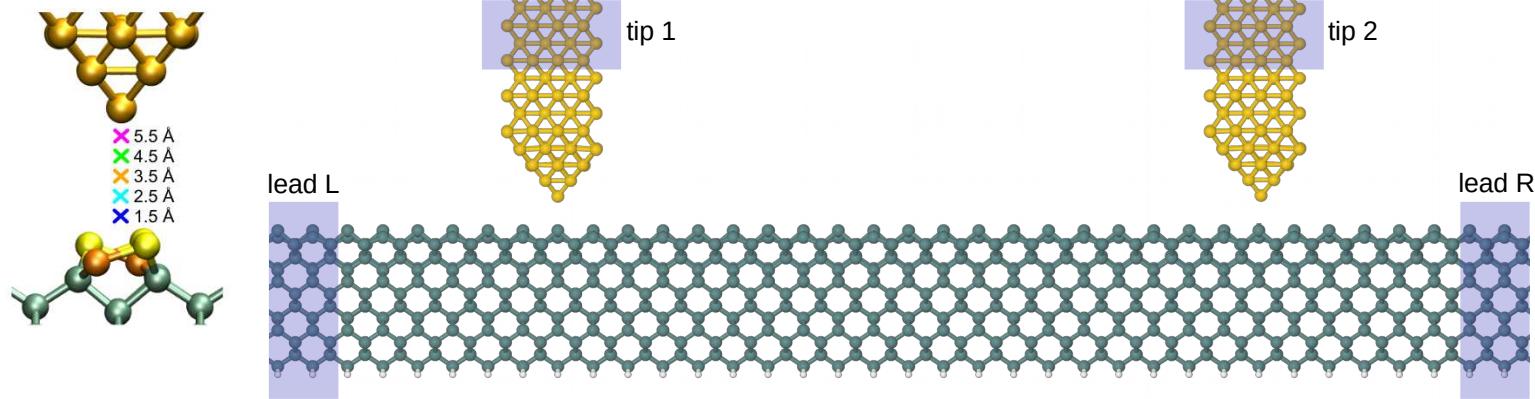
Ge(001) surface addressed by two tips: 4-terminal setup



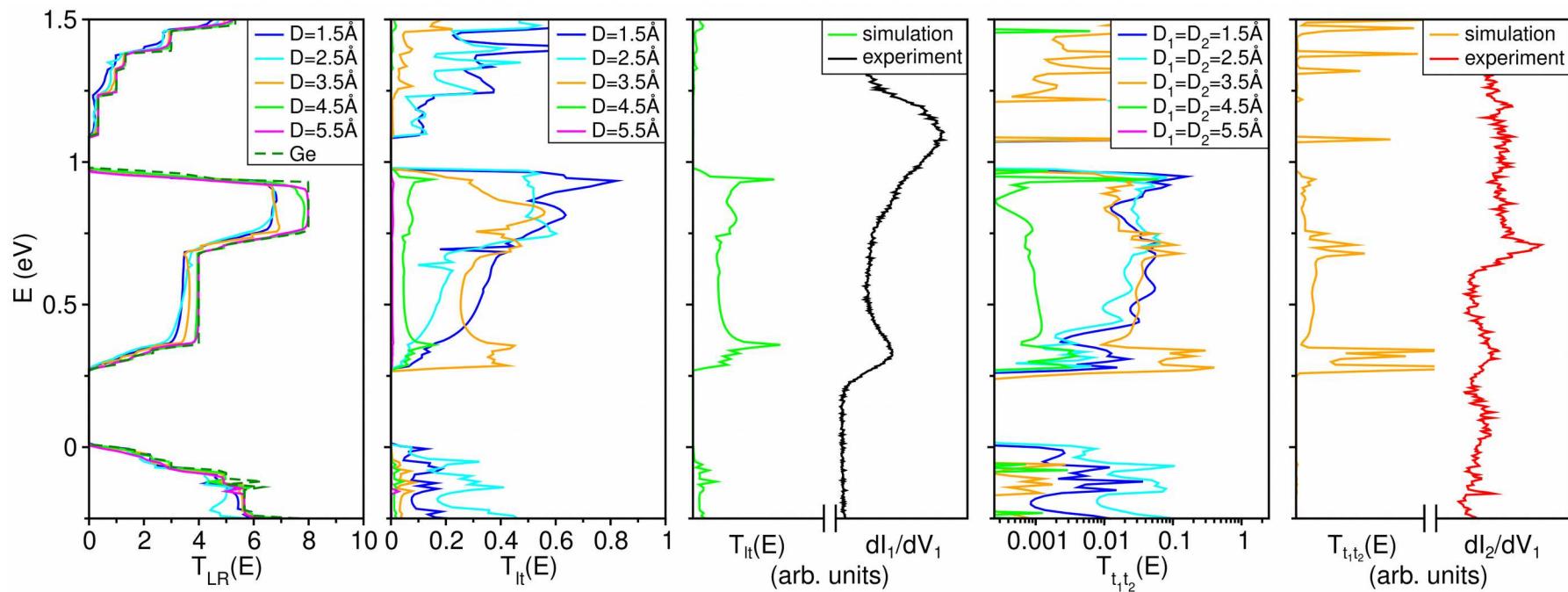
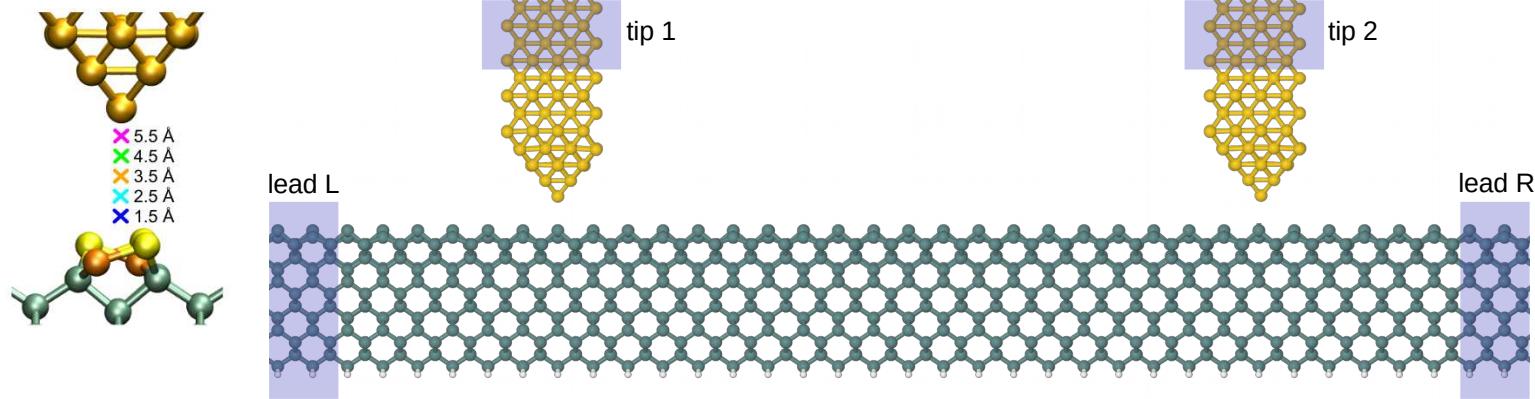
Ge(001) surface addressed by two tips: 4-terminal setup



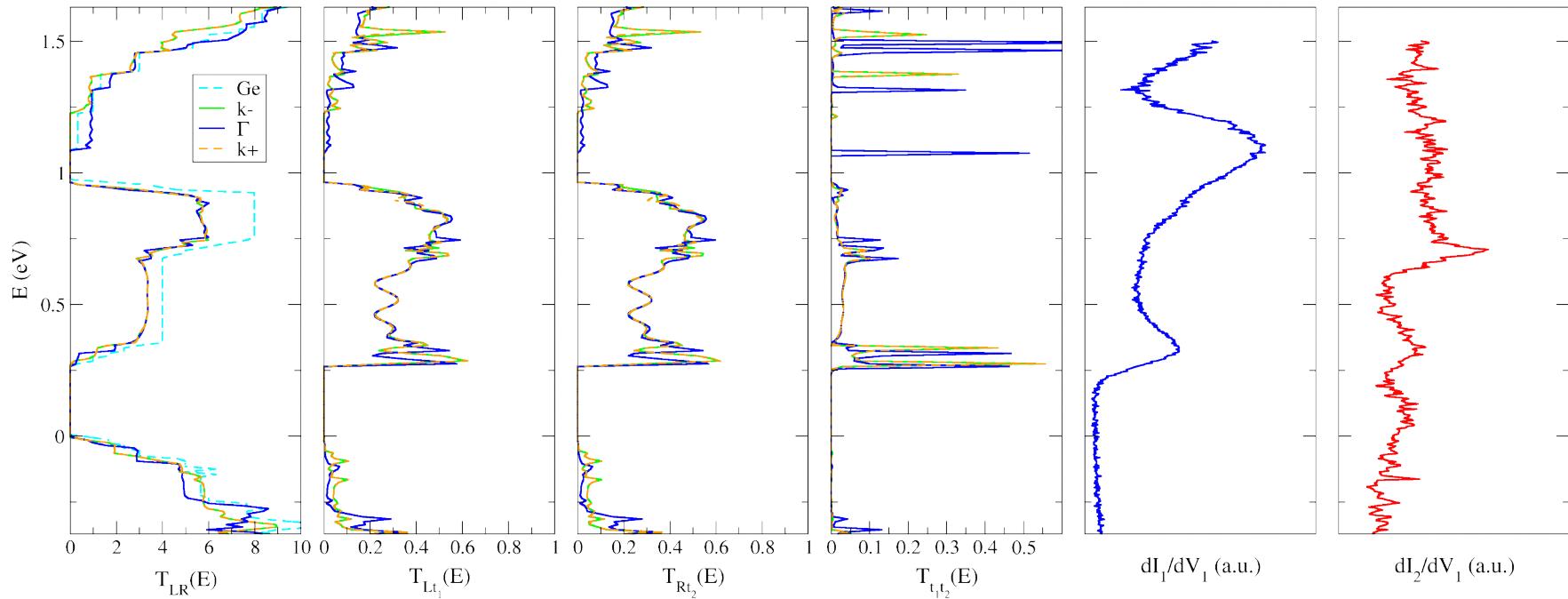
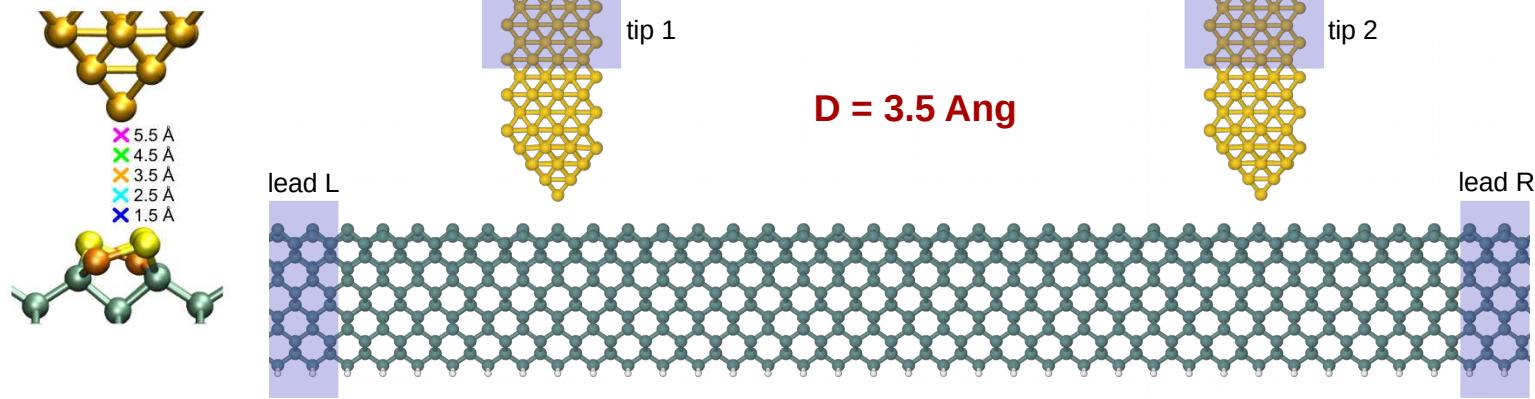
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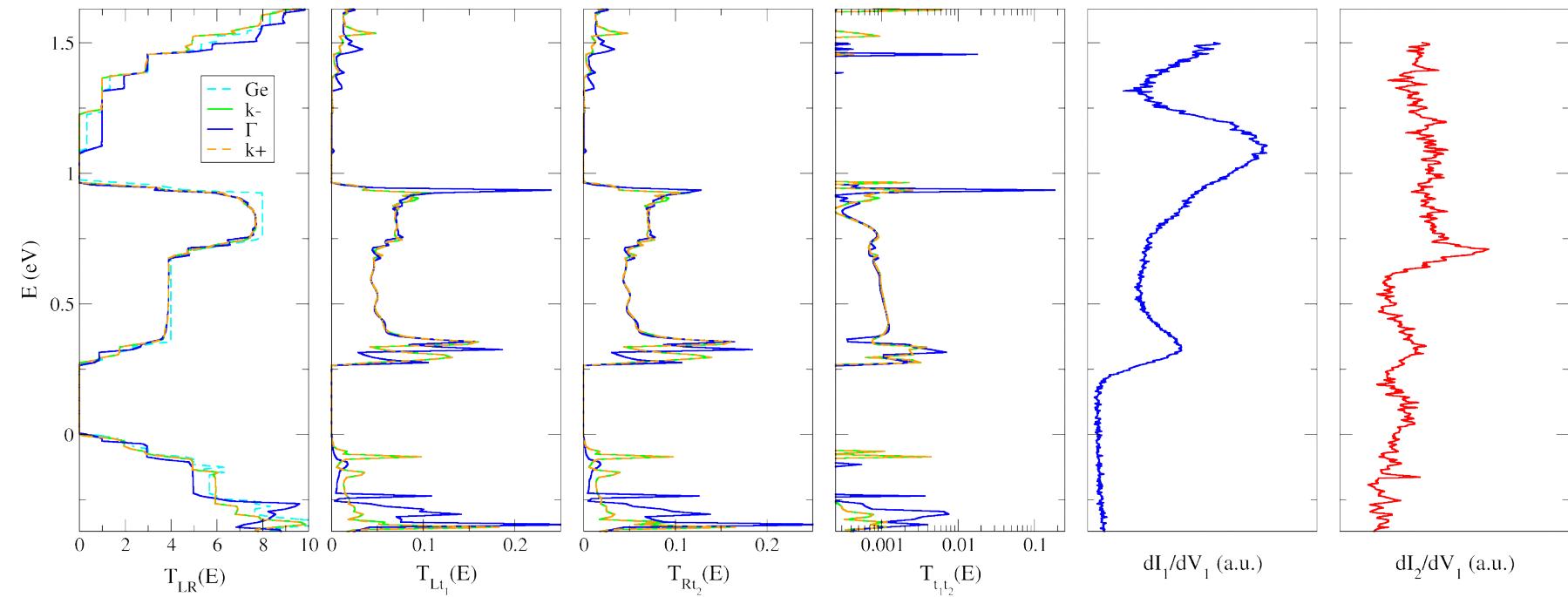
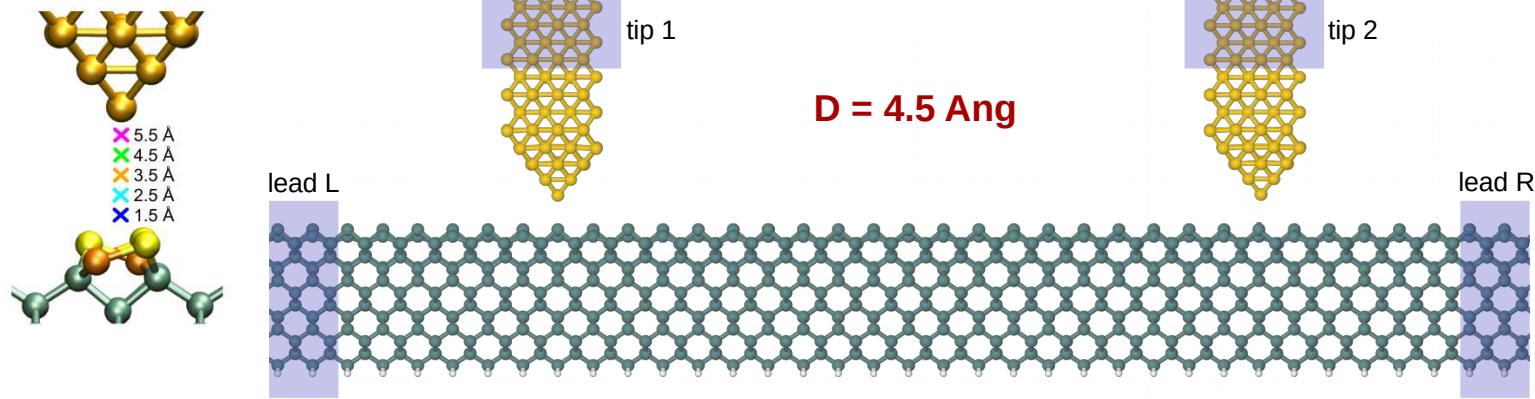
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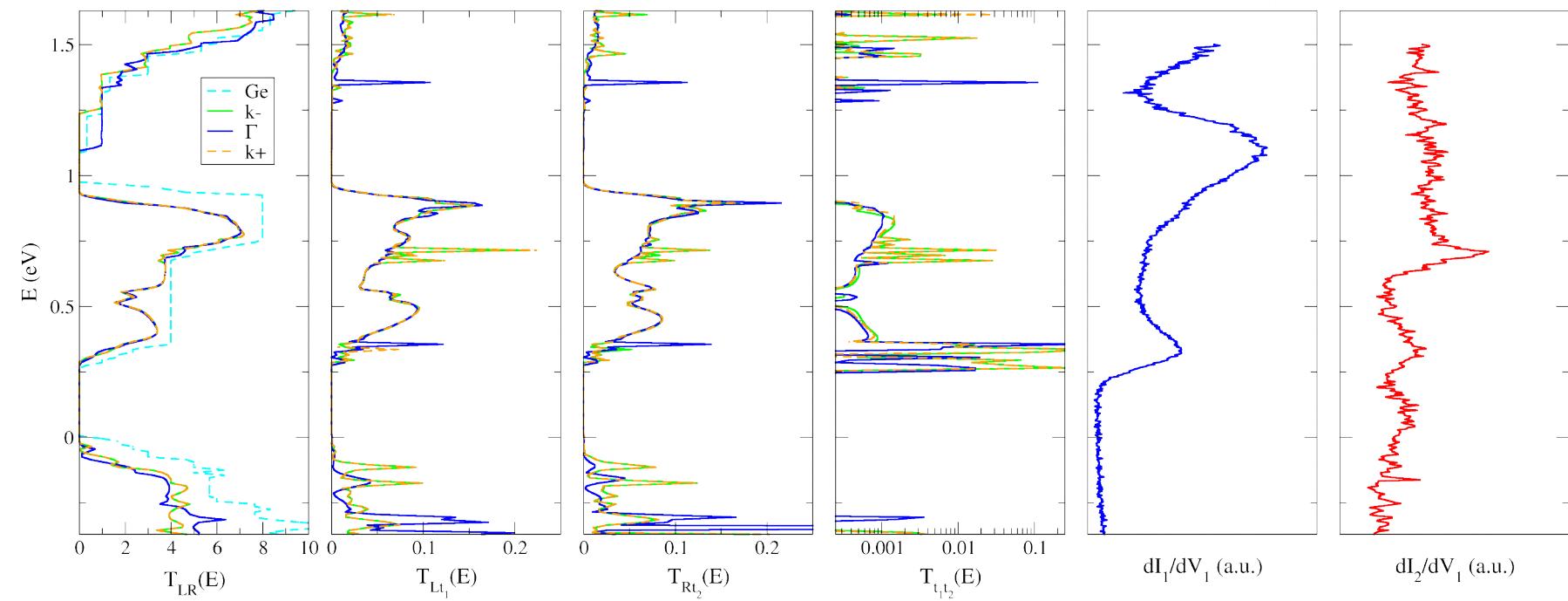
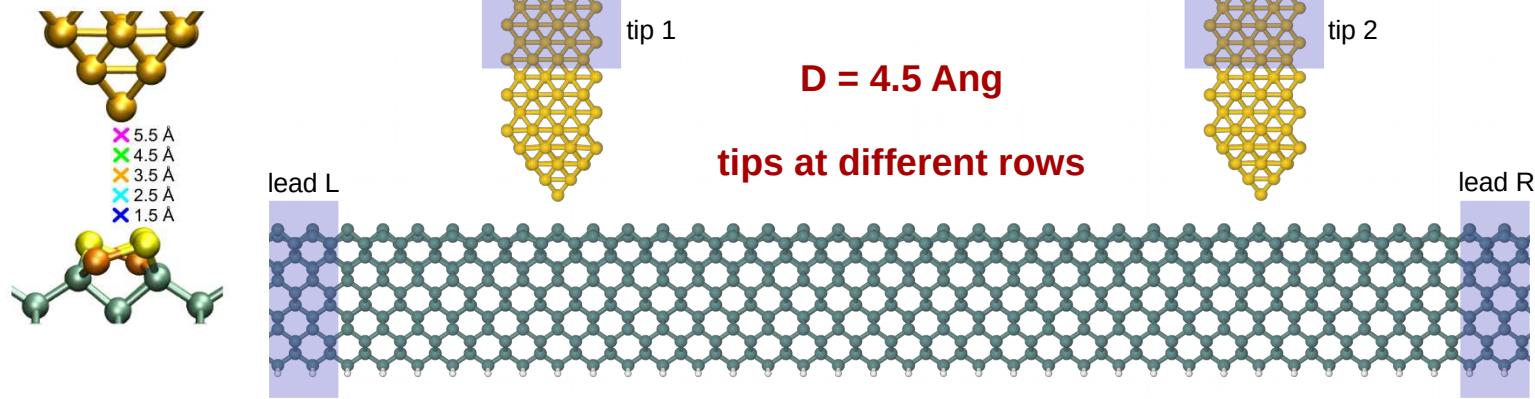
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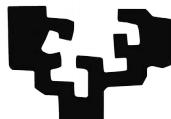


Ge(001) surface addressed by two tips: 4-terminal setup



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!



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