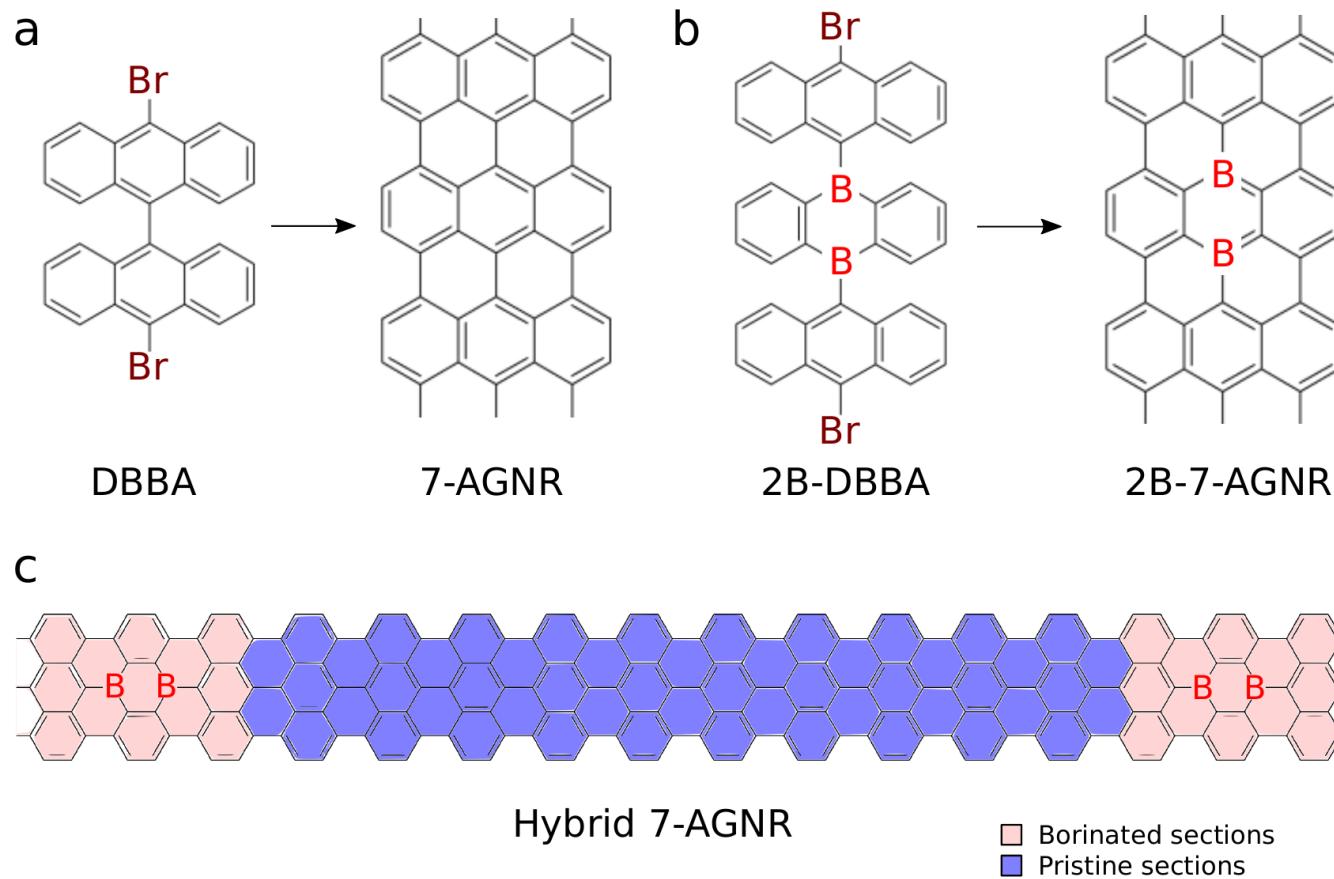




1-D Quantum Well States on Doped Graphene Nanoribbons Revealed by Transport Simulations

Pedro Brandimarte, Aran Garcia-Lekue, Mads Engelund,
Thomas Frederiksen and Daniel Sánchez-Portal

May 26, 2016



S. Kawai *et al.* *Nature Communications* **6**, 8098 (2015).

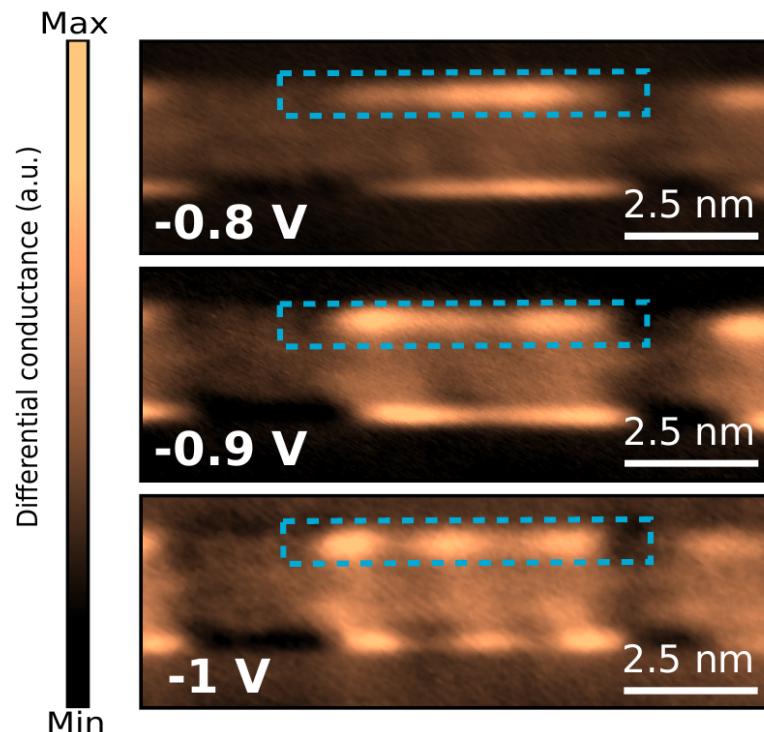
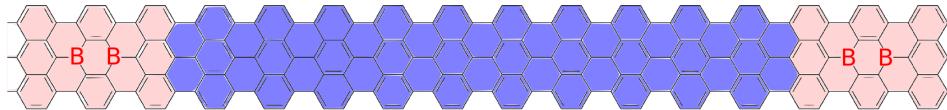
R. R. Cloke *et al.* *J. A. Chem. Soc.* **137**, 8872 (2015).



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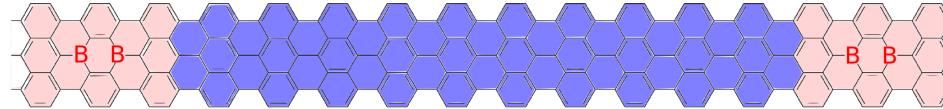
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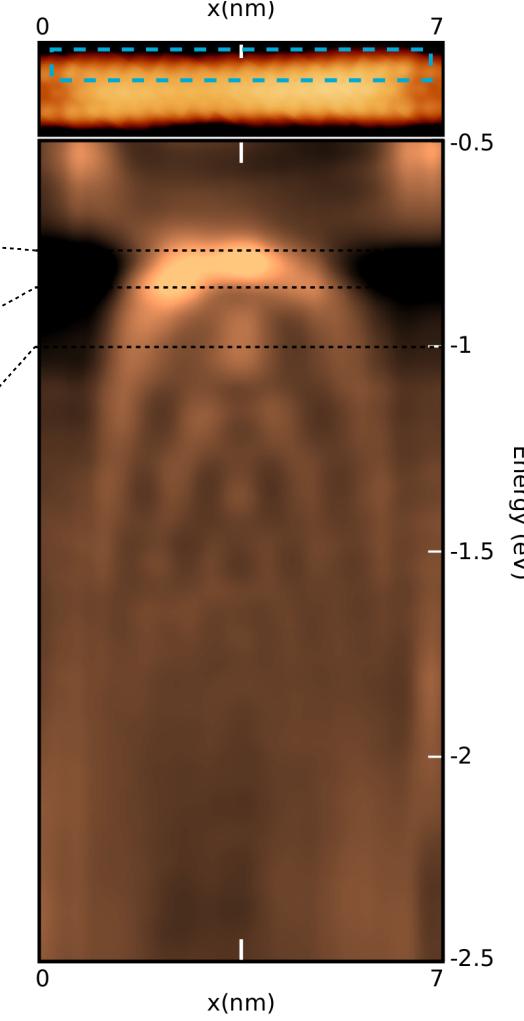
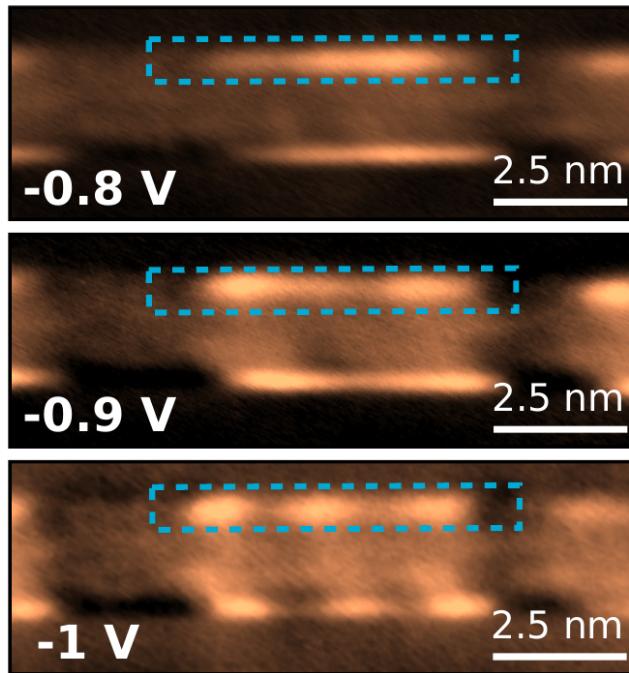
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Max

Differential conductance (a.u.)

Min



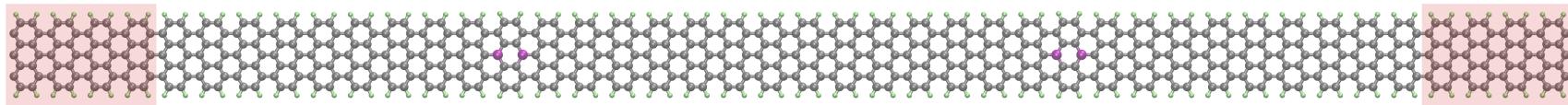


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TranSIESTA





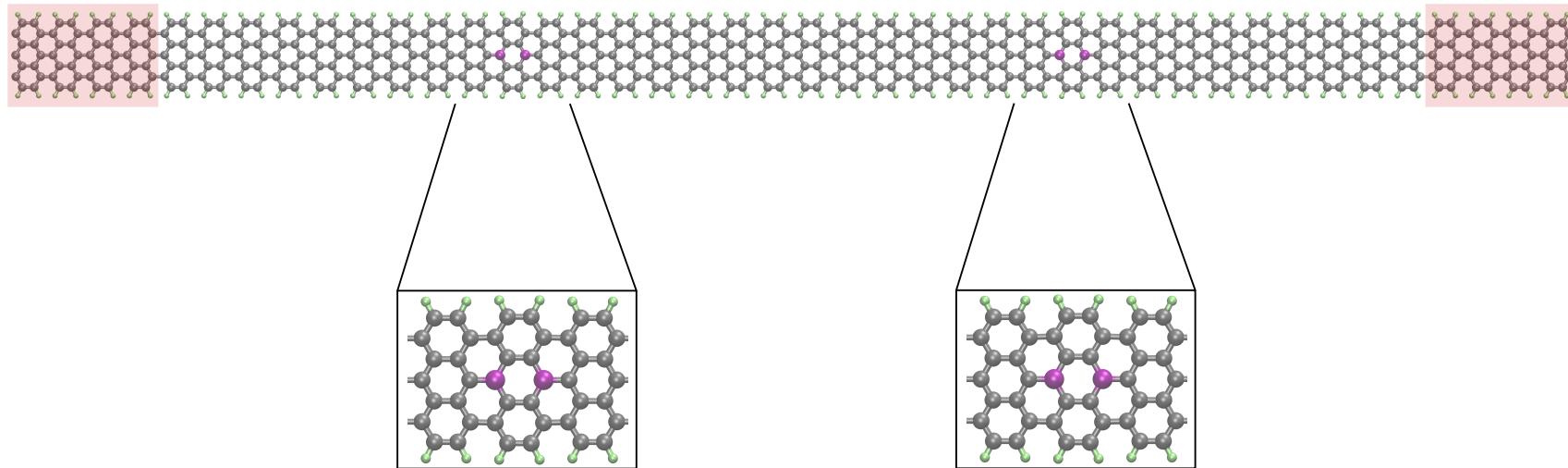
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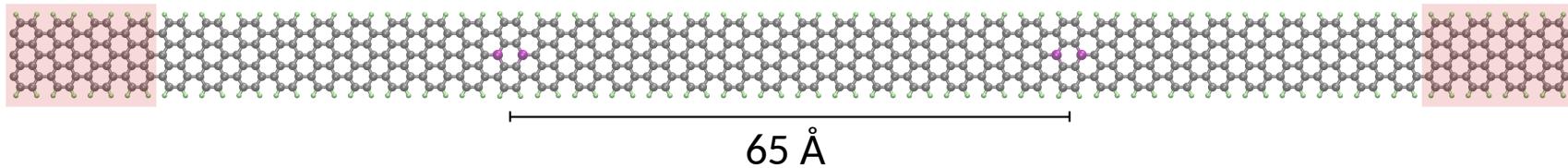


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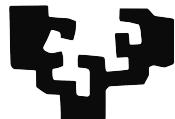


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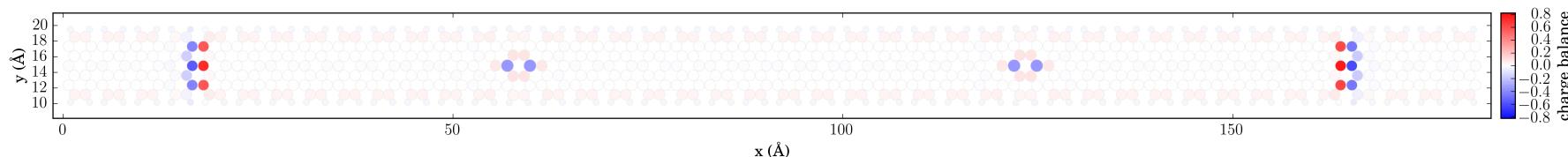
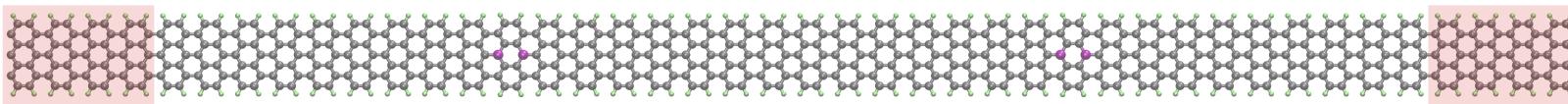


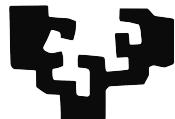
Simulation characteristics:

- 756 atoms;
- double- ζ (5040 orbitals);
- vdW (optB88);
- real space grid cutoff: 250 Ry;
- forces < 10 meV/ \AA .

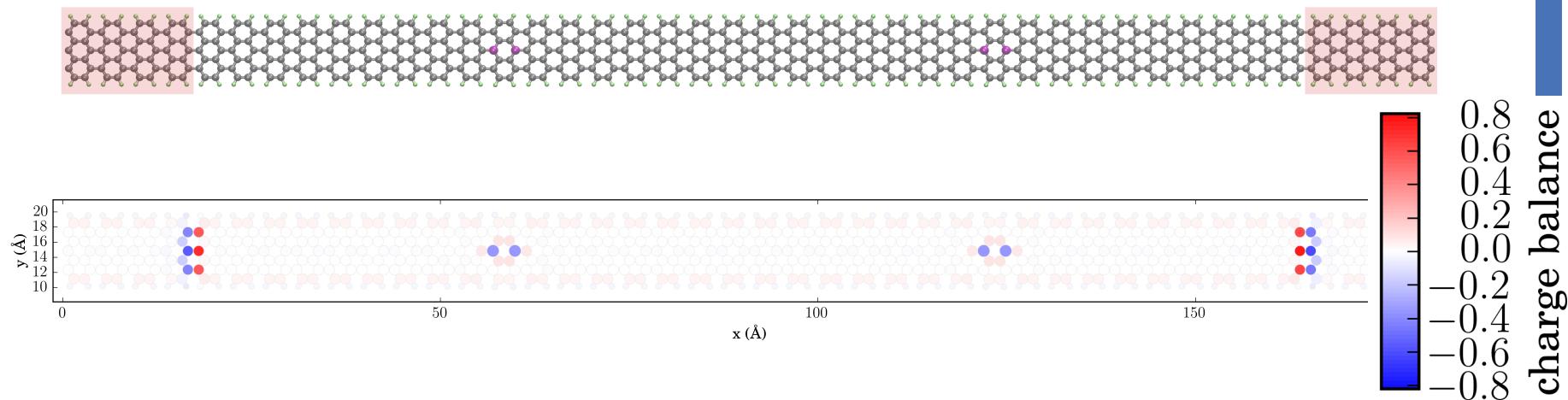


Mulliken population



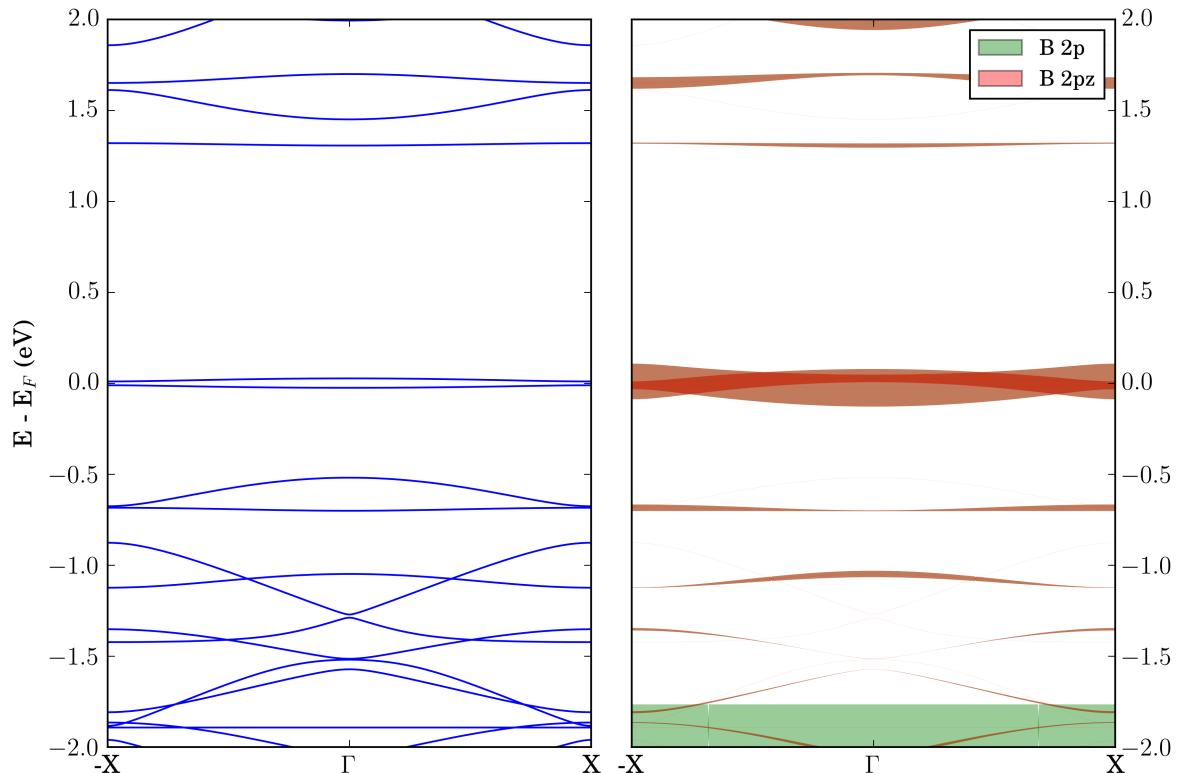
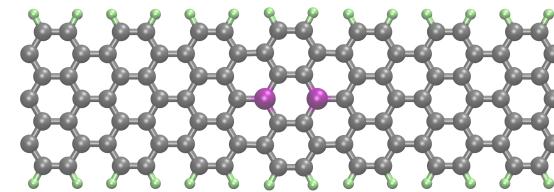


Mulliken population



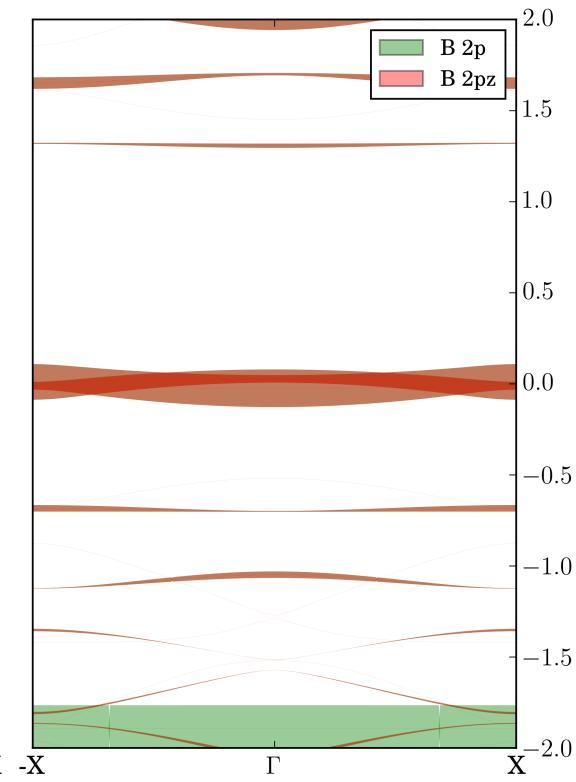
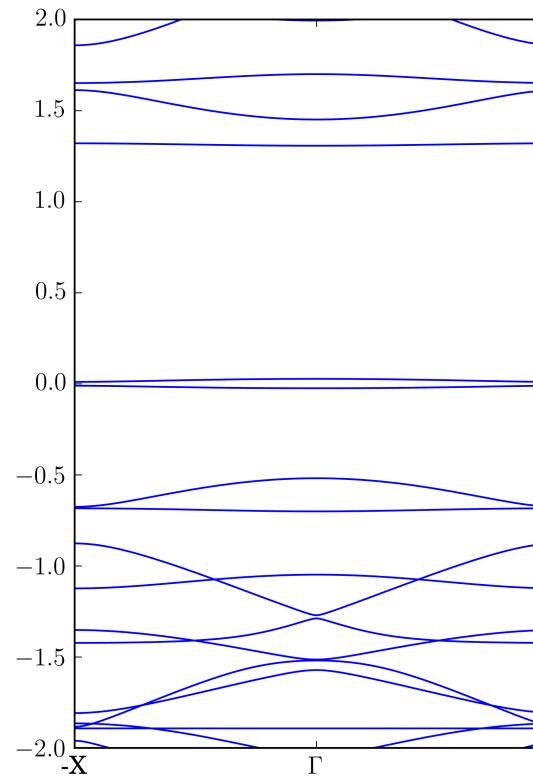
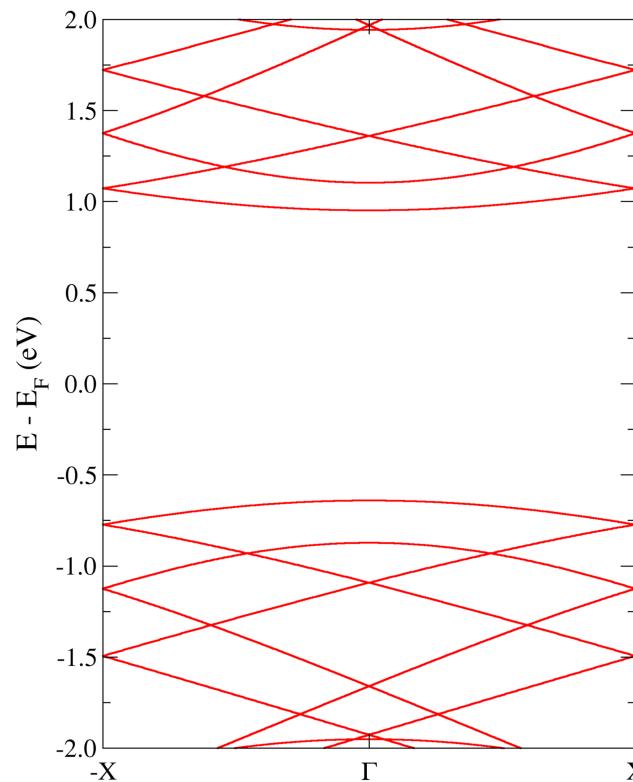
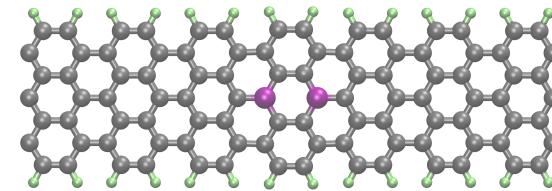
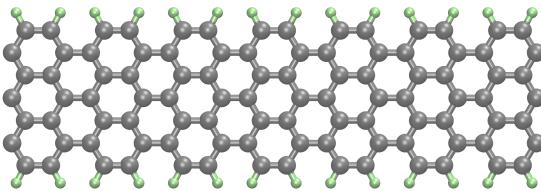


Periodic calculation



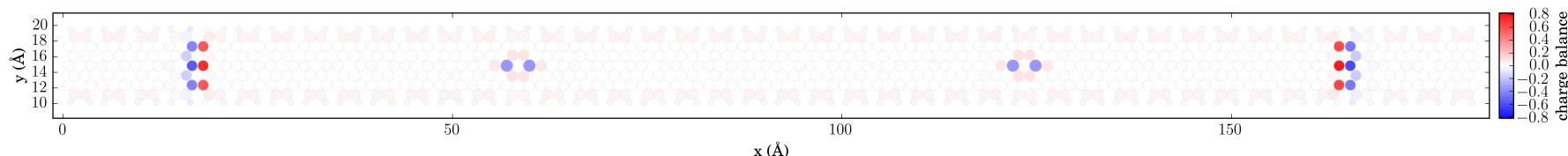
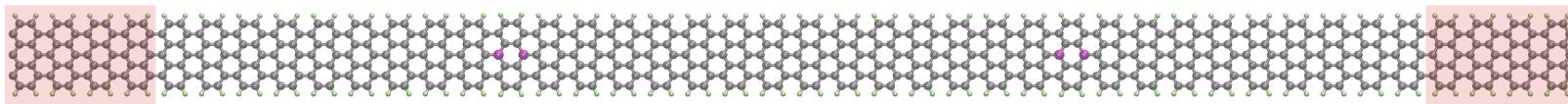


Periodic calculation





Mulliken population





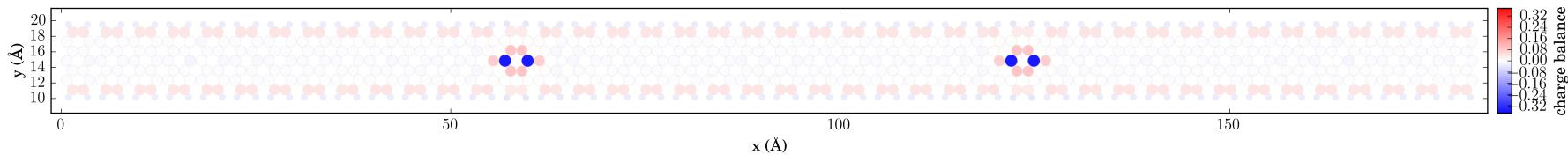
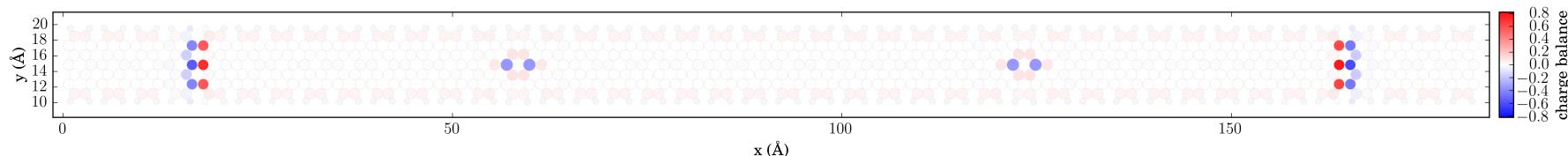
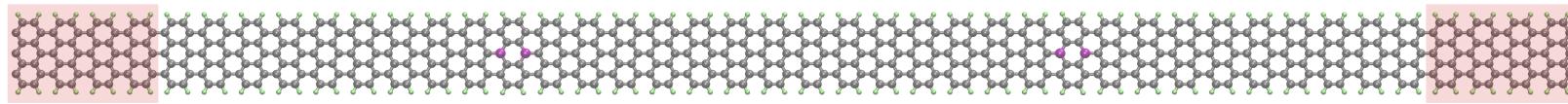
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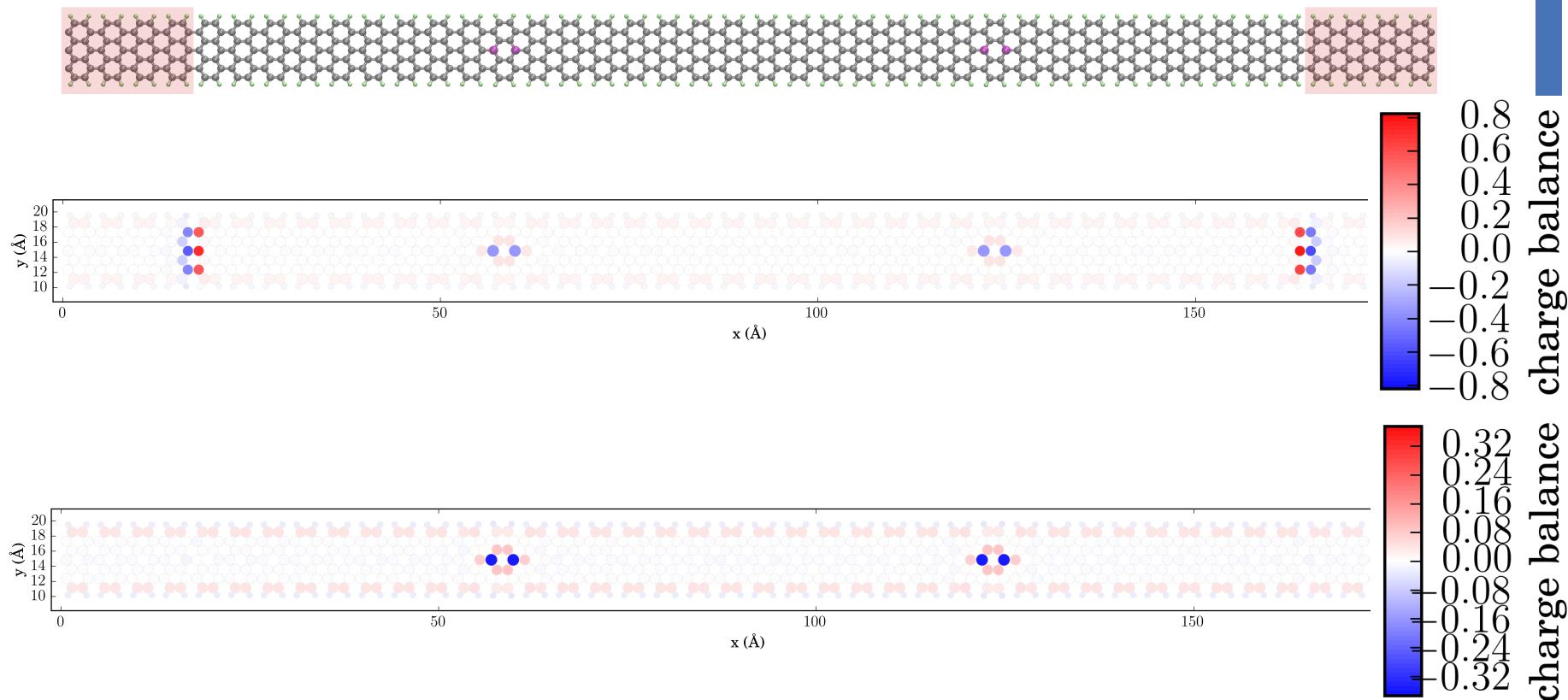


Mulliken population



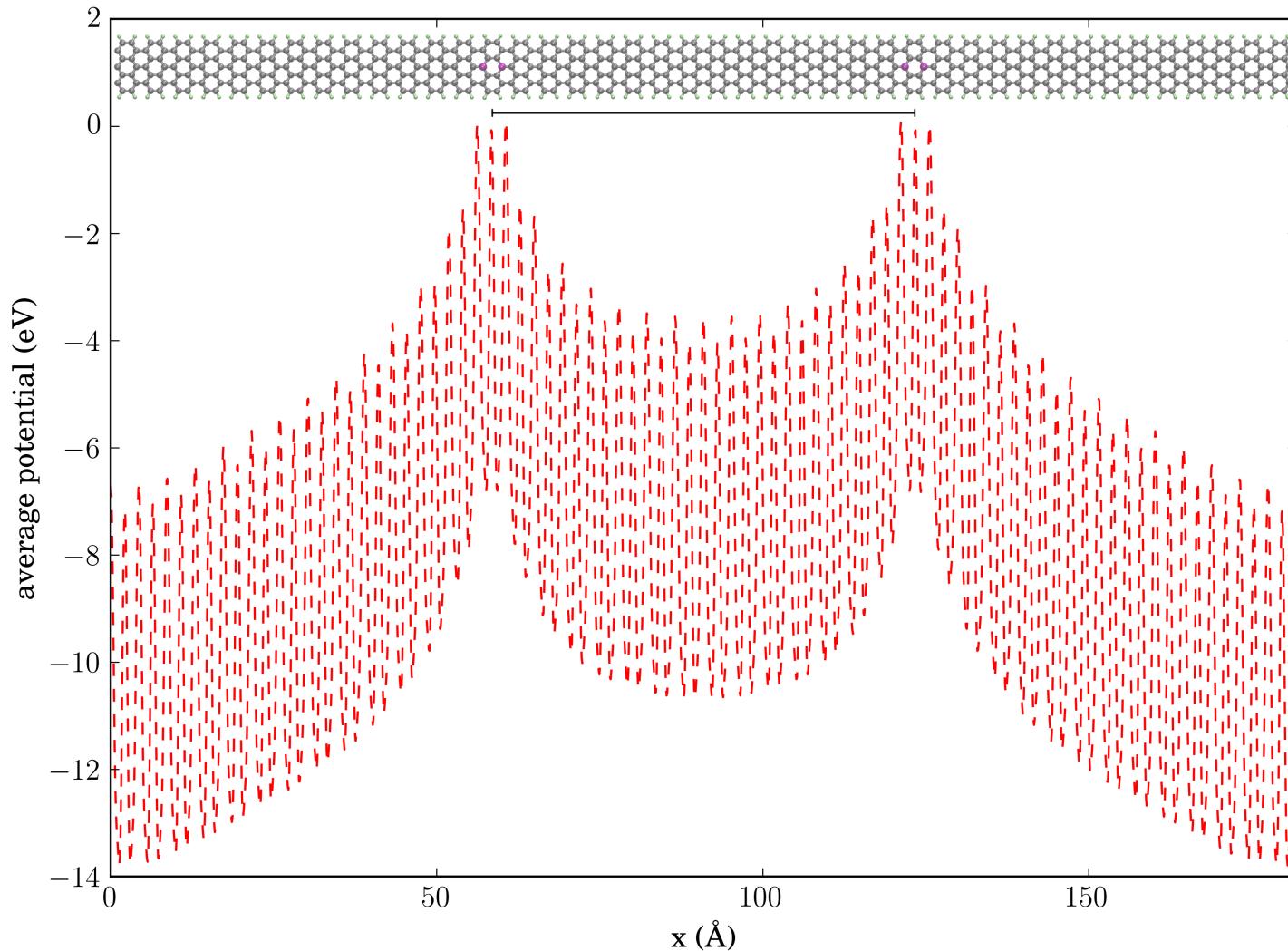


Mulliken population



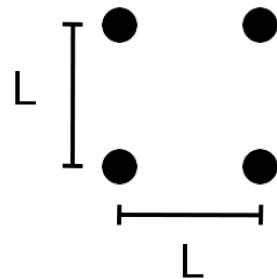


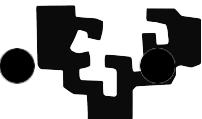
Electrostatic potential



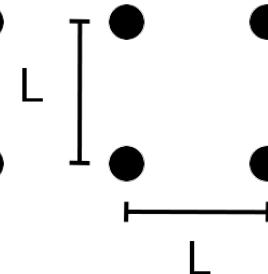


Supercell approach



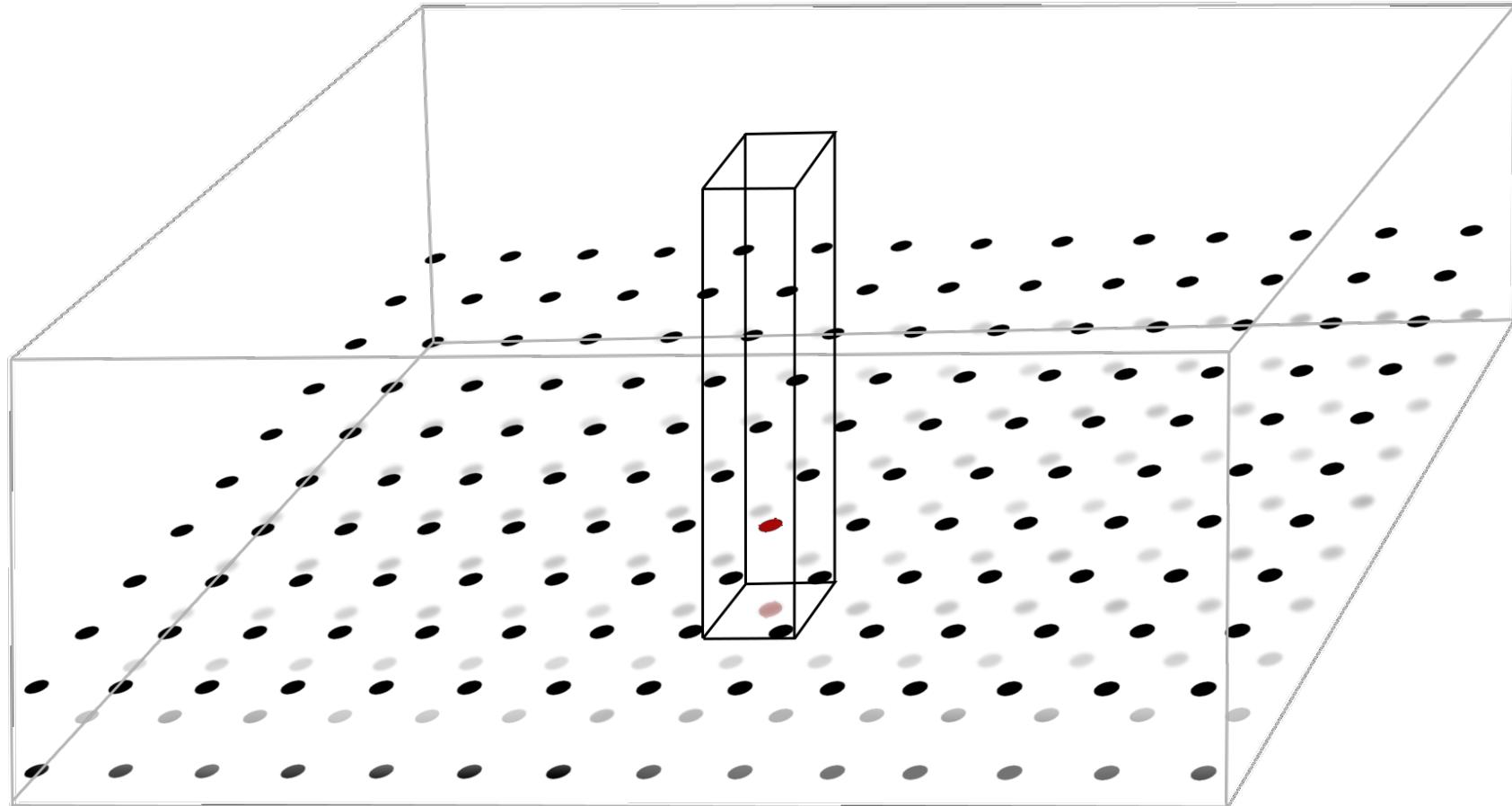


Supercell approach



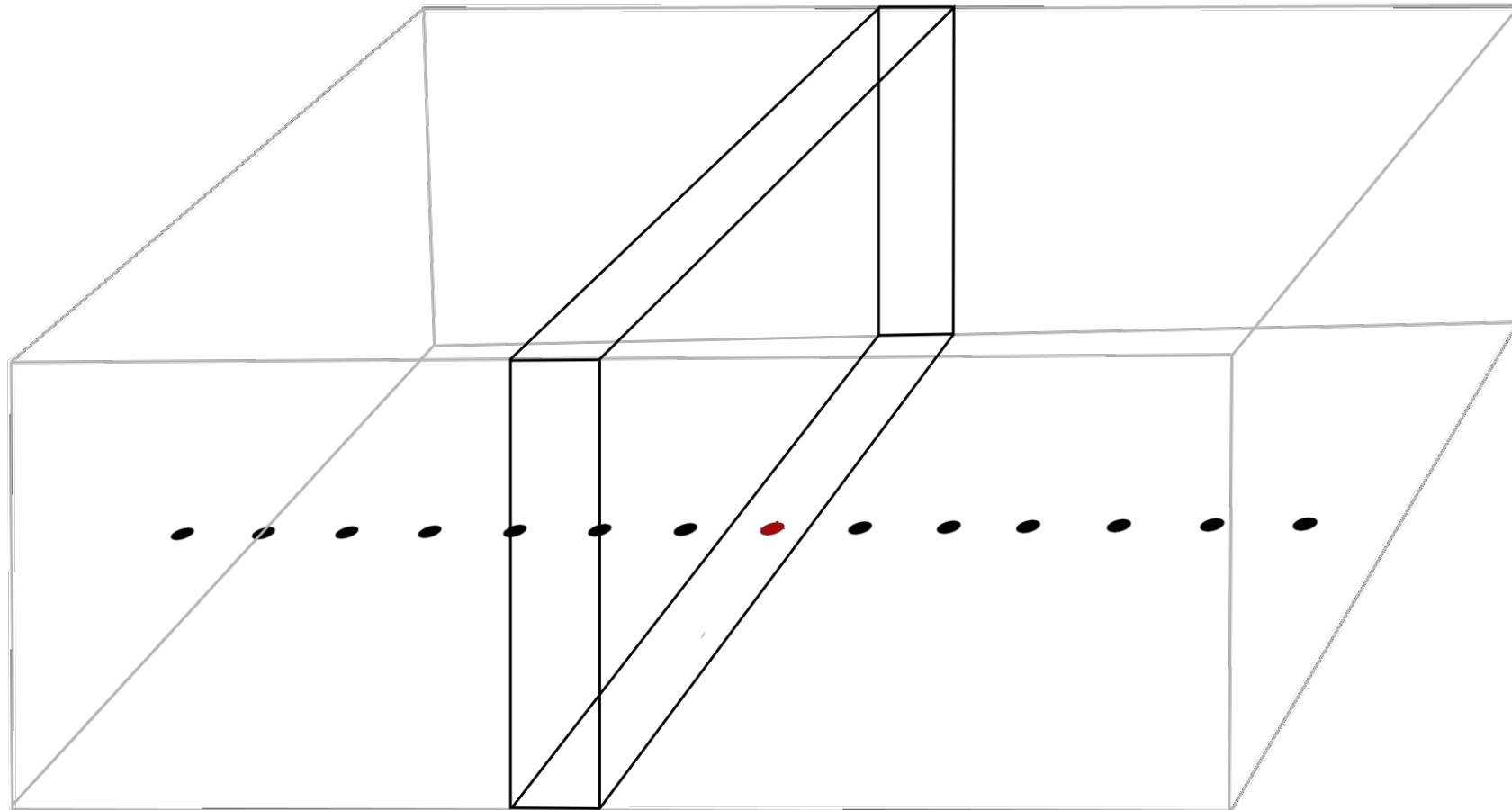


Supercell approach





Supercell approach





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Coulomb cutoff

$$\nabla^2 V(\mathbf{r}) = -4\pi n(\mathbf{r})$$



Coulomb cutoff

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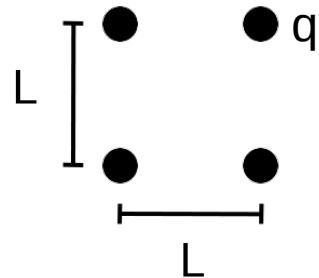


$$V(\mathbf{r}) = \int \int \int_{space} \frac{n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d^3 \mathbf{r}'$$



Coulomb cutoff

$$\nabla^2 V(\mathbf{r}) = -4\pi n(\mathbf{r}) \quad \longrightarrow \quad V(\mathbf{r}) = \int \int \int_{space} \frac{n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d^3 \mathbf{r}'$$



$$V(\mathbf{r}) = \sum_{\{\mathbf{L}\}} \frac{q}{|\mathbf{r} - \mathbf{L}|}$$



Coulomb cutoff

$$\nabla^2 V(\mathbf{r}) = -4\pi n(\mathbf{r})$$



$$V(\mathbf{r}) = \int \int \int_{space} \frac{n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d^3 \mathbf{r}'$$

$$V(\mathbf{G}) = n(\mathbf{G})v(\mathbf{G}), \quad v(\mathbf{G}) = \frac{4\pi}{G^2}$$



Coulomb cutoff

$$\nabla^2 V(\mathbf{r}) = -4\pi n(\mathbf{r}) \quad \longrightarrow \quad V(\mathbf{r}) = \int \int \int_{space} \frac{n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d^3 \mathbf{r}'$$

$$V(\mathbf{G}) = n(\mathbf{G})v(\mathbf{G}), \quad v(\mathbf{G}) = \frac{4\pi}{G^2}$$

$$V(\mathbf{r}) = \frac{4\pi}{\Omega} \sum_{\mathbf{G} \neq 0} \frac{n(\mathbf{G})}{G^2} \exp(i\mathbf{G} \cdot \mathbf{r})$$



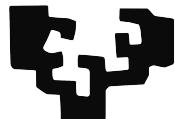
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Coulomb cutoff

$$\tilde{v}(\mathbf{G}) = \int \int \int_{space} \tilde{v}(r) e^{-i\mathbf{G} \cdot \mathbf{r}} d^3 \mathbf{r} = \int \int \int_{\mathcal{D}} v(r) e^{-i\mathbf{G} \cdot \mathbf{r}} d^3 \mathbf{r}$$



Coulomb cutoff

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- 0-D: $\tilde{v}^{0D}(G) = \frac{4\pi}{G^2} [1 - \cos(GR)]$



Coulomb cutoff

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- 0-D: $\tilde{v}^{0D}(G) = \frac{4\pi}{G^2} [1 - \cos(GR)]$
- 1-D: $\tilde{v}^{1D}(G_x, G_{\perp}) = \frac{4\pi}{G^2} [1 + G_{\perp} R J_1(G_{\perp} R) K_0(G_x R) - G_x R J_0(G_{\perp} R) K_1(G_x R)]$



Coulomb cutoff

$$\tilde{v}(\mathbf{G}) = \int \int \int_{space} \tilde{v}(r) e^{-i\mathbf{G} \cdot \mathbf{r}} d^3 \mathbf{r} = \int \int \int_{\mathcal{D}} v(r) e^{-i\mathbf{G} \cdot \mathbf{r}} d^3 \mathbf{r}$$

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$$\approx -4\pi \int_0^R r J_0(G_\perp r) \ln(r) dr + 4\pi R \ln(2h) \frac{J_1(G_\perp R)}{G_\perp}$$



Coulomb cutoff

$$\tilde{v}(\mathbf{G}) = \int \int \int_{space} \tilde{v}(r) e^{-i\mathbf{G} \cdot \mathbf{r}} d^3 \mathbf{r} = \int \int \int_{\mathcal{D}} v(r) e^{-i\mathbf{G} \cdot \mathbf{r}} d^3 \mathbf{r}$$

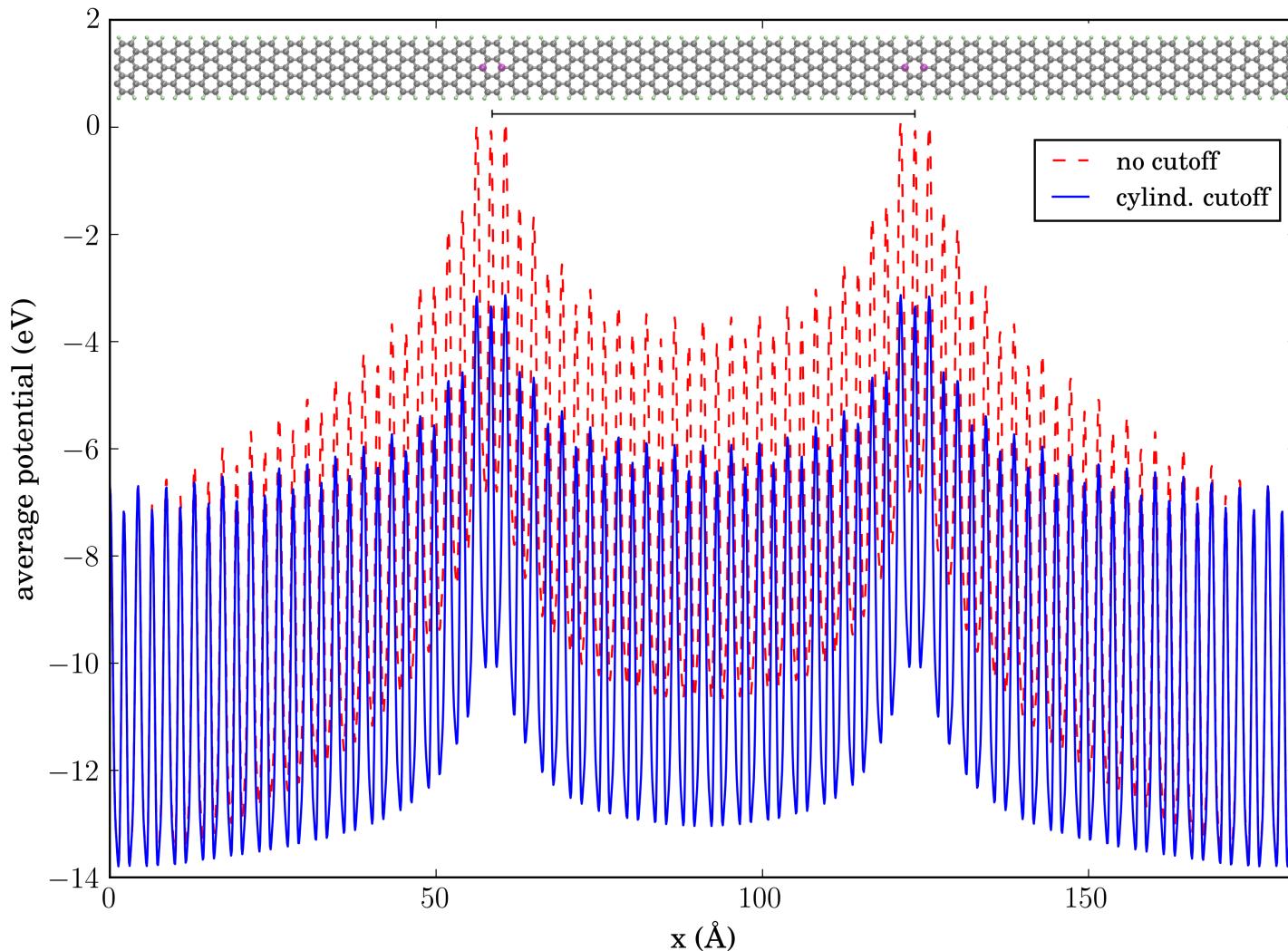
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$= 0$

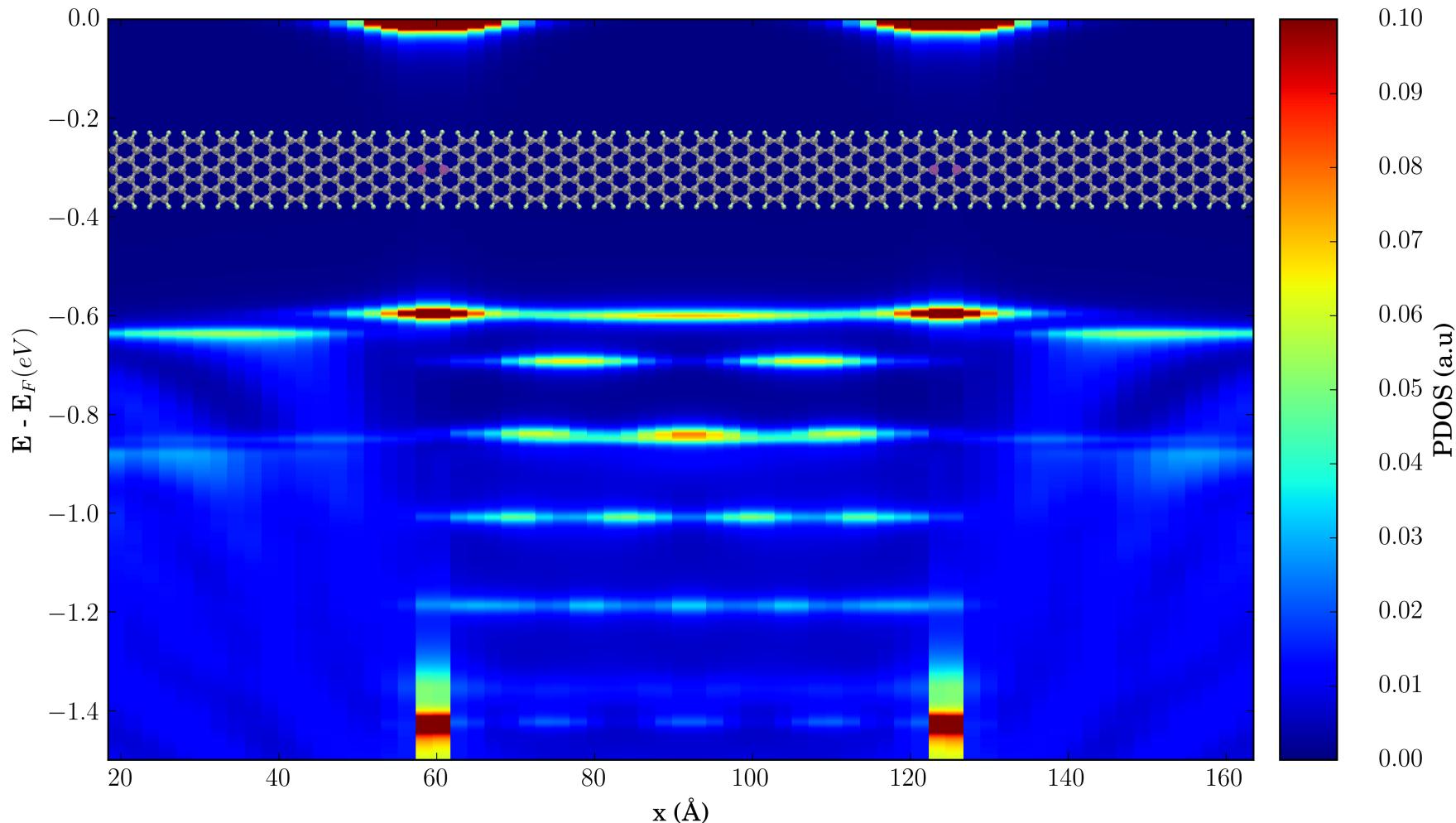


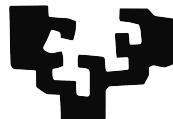
Electrostatic potential



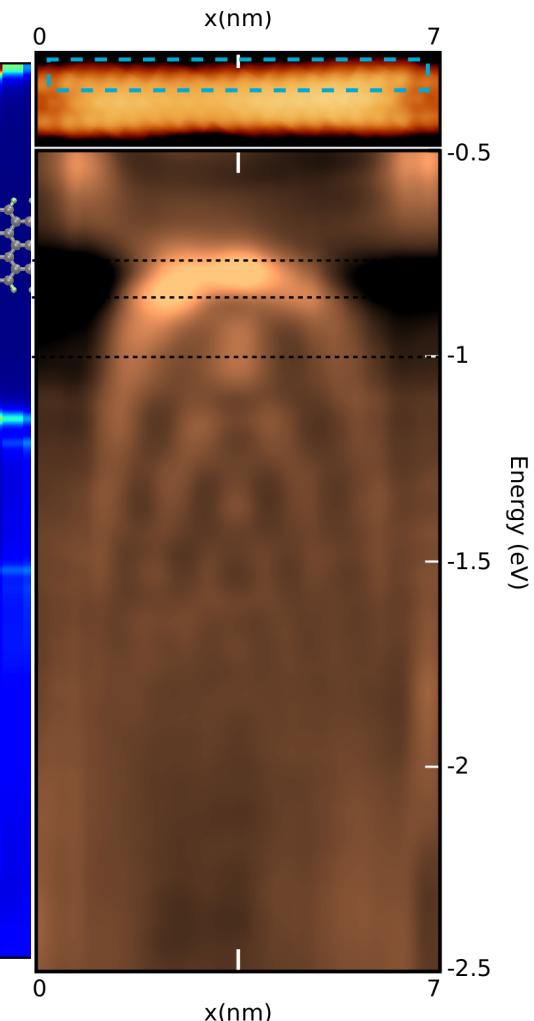
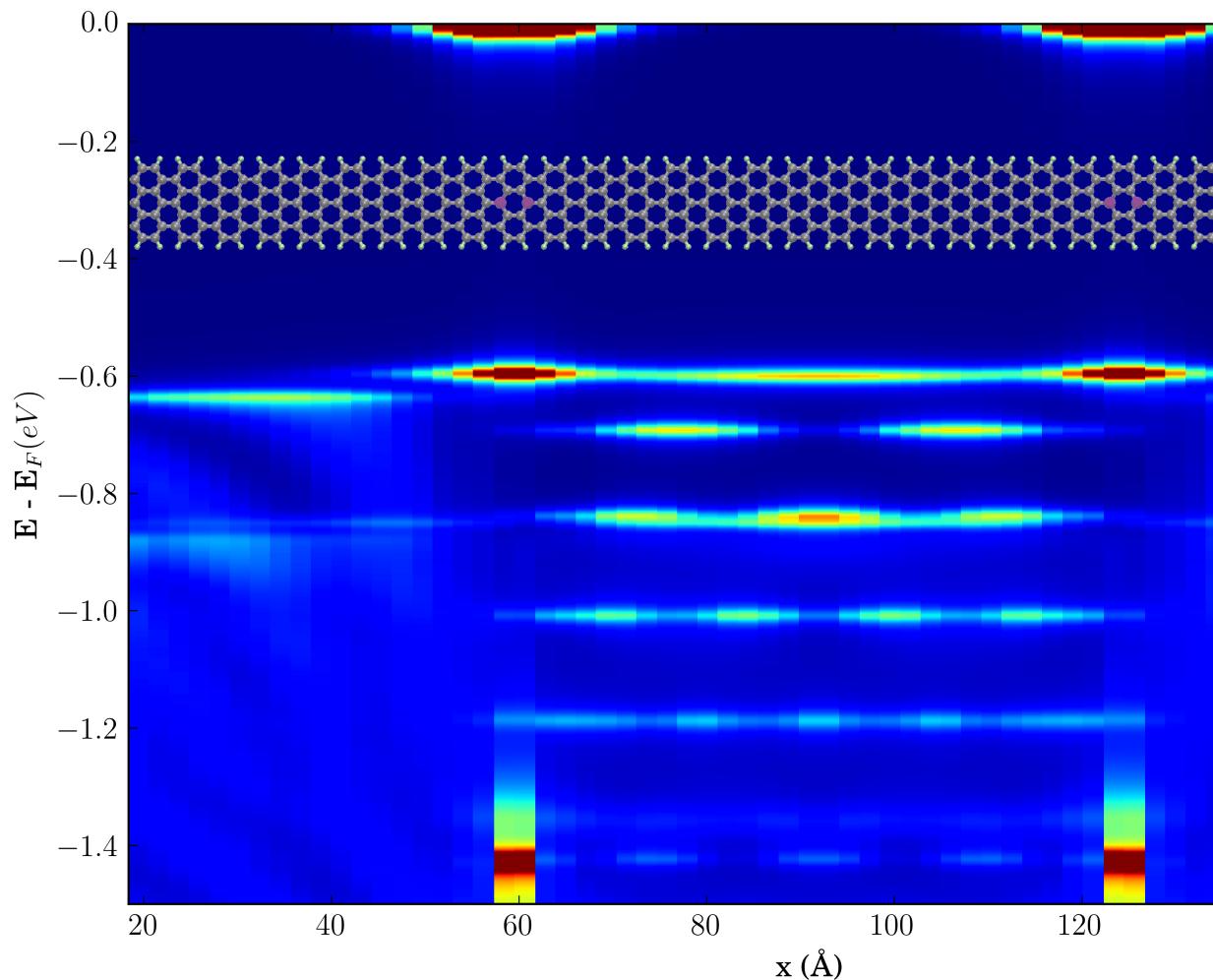


DOS projected on each ribbon “row”





DOS projected on each ribbon “row”





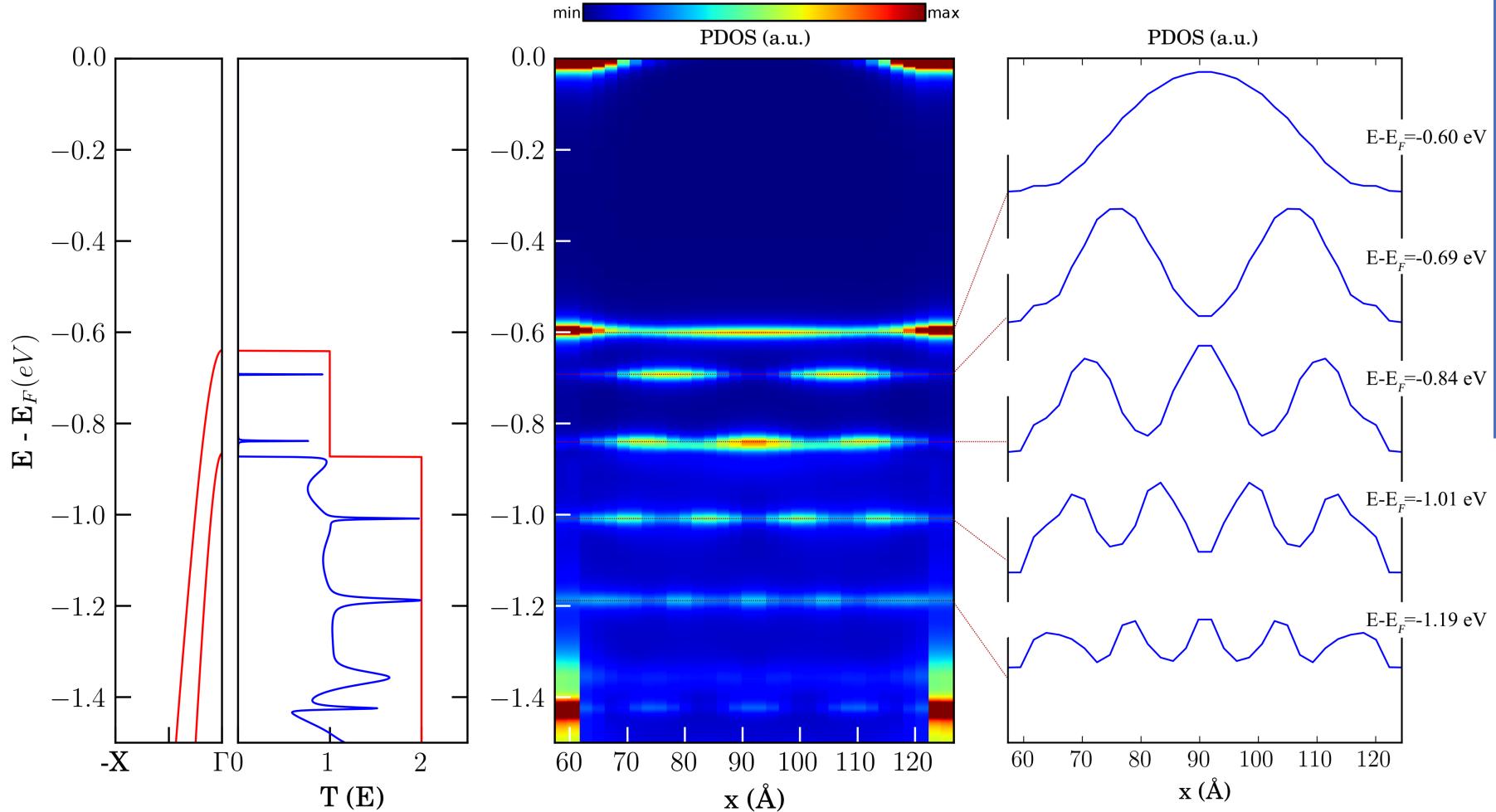
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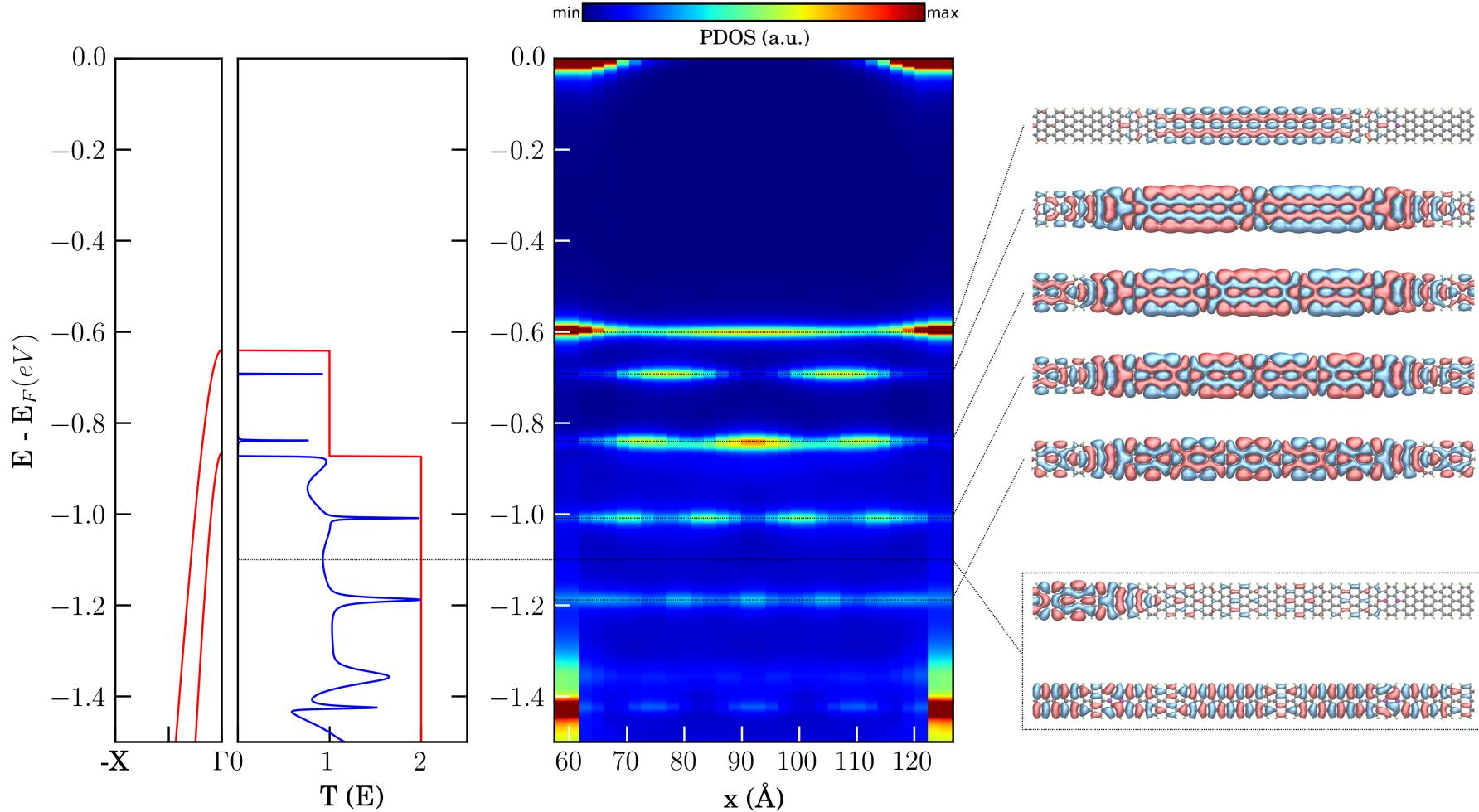
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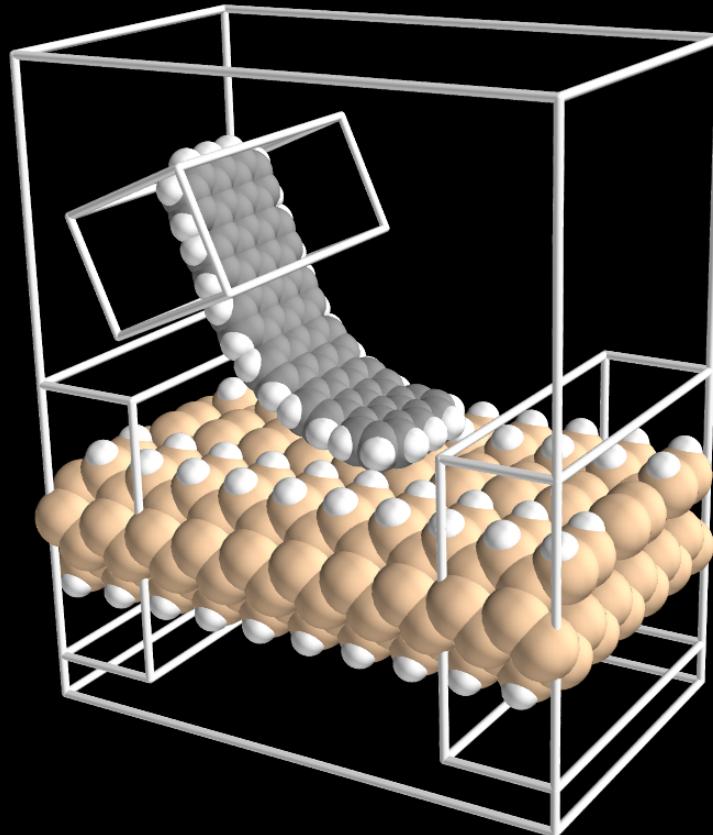


Conclusions

- Semiconductor electrodes: **use with caution!**
- **Coulomb cutoff in TranSIESTA** for low dimensionality systems;
- Transport simulations can **reproduce** observed quantum well states and **explain** their mechanism.



On going simulations





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Thank you!



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