

Investigation of the electronic structure and of electronic currents in graphene antidote lattices

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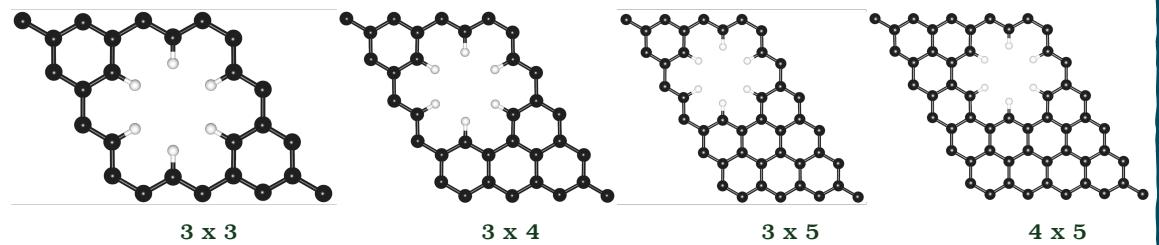


Graphene Antidot Lattices (GALs)

Goal: New graphene-based materials for electronic devices

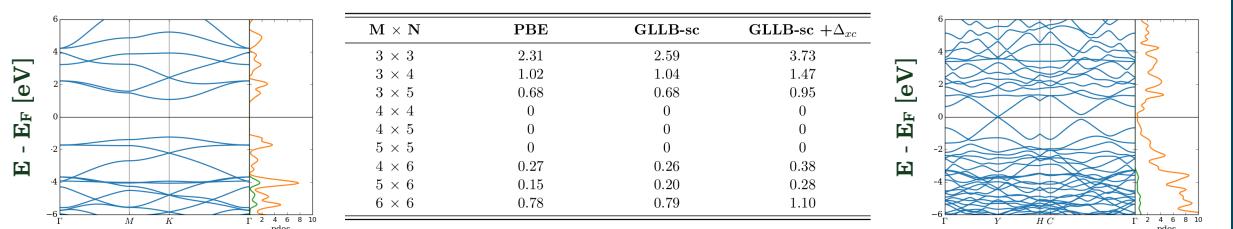
Requirements and observations:

- Suitable band gap
- Highly dependent on symmetry and size of the unit cell
- Hydrogen passivated GALs more suitable

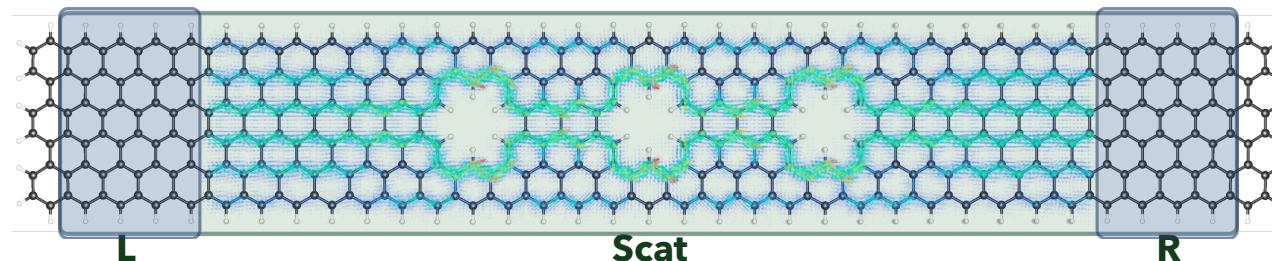


Methods:

- Electronic structures employing DFT^[1] functionals.
- Precise band gap employing GLLB-SC and GOWO.^[1]



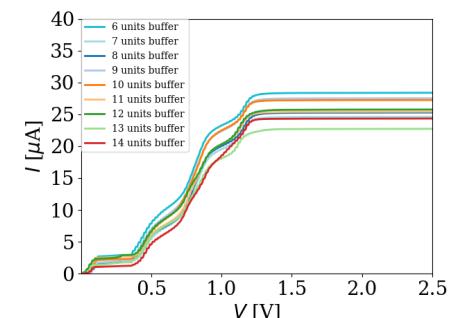
Electronic Transport Model



Methods:

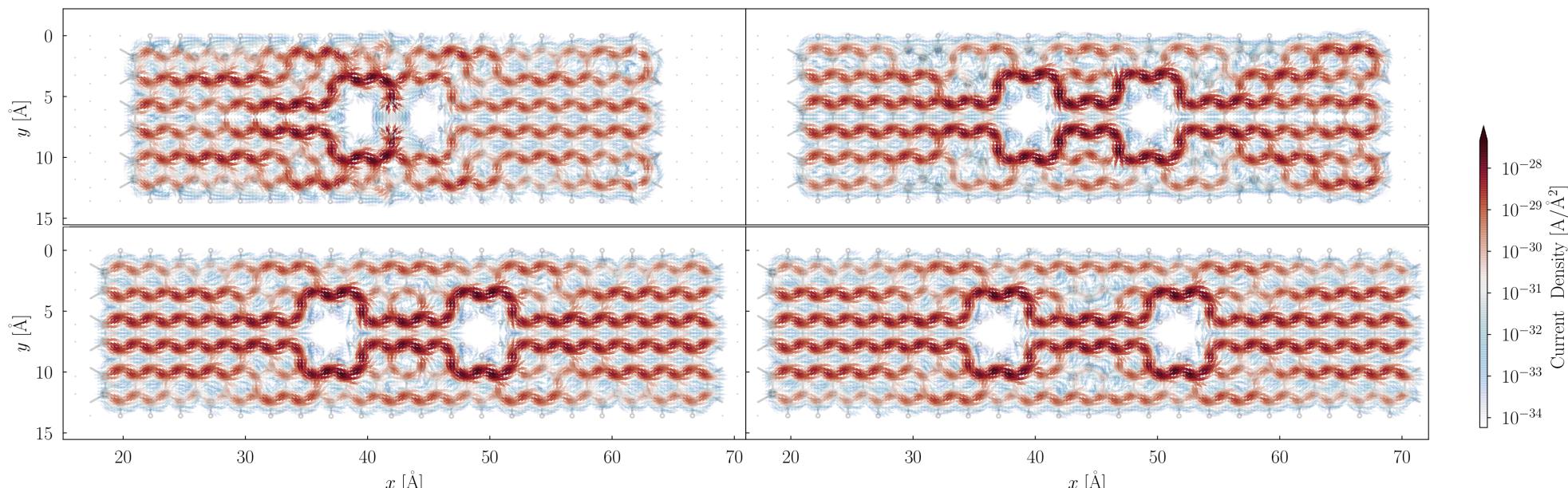
- Scattering region connected to two semi-infinite leads.
- Enough buffer region in order to avoid interaction between leads L and leads R.
- Avoiding edge effect by removing the edge of a saturated molecular structure.
- Transmission function is calculated via NEGFs approach as implemented in ASE package^[2].
- Voltage dependent current is obtained with standard Landauer Equation.

$$H = \begin{pmatrix} \dots & V_{LL} & 0 & 0 & 0 & 0 & 0 \\ V_{LL} & H_L & V_{LL} & 0 & 0 & 0 & 0 \\ 0 & V_{LL} & H_L & \tau_L & 0 & 0 & 0 \\ 0 & 0 & \tau_L^+ & H_{scat} & \tau_R & 0 & 0 \\ 0 & 0 & 0 & \tau_R^+ & H_R & V_{RR} & 0 \\ 0 & 0 & 0 & 0 & V_{RR} & H_R & V_{RR} \\ 0 & 0 & 0 & 0 & 0 & V_{RR} & \dots \end{pmatrix}$$



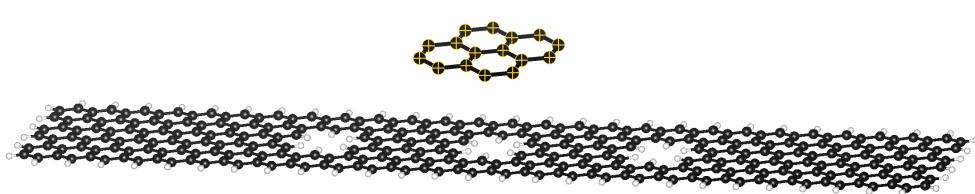
Electronic Current Flux Density

Mapping the current density on a spatial grid based on NEGF results^[3]



Outlook

- Influence of the width of the ZGNRs
- Influence of a small organic molecule on the current density when placed it on top



References and Acknowledgement

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3. M. Walz, A. Bagrets, F. Evers; *JCTC*. 2015
4.
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