Graphine on SiO2, Transport in FHI-aims

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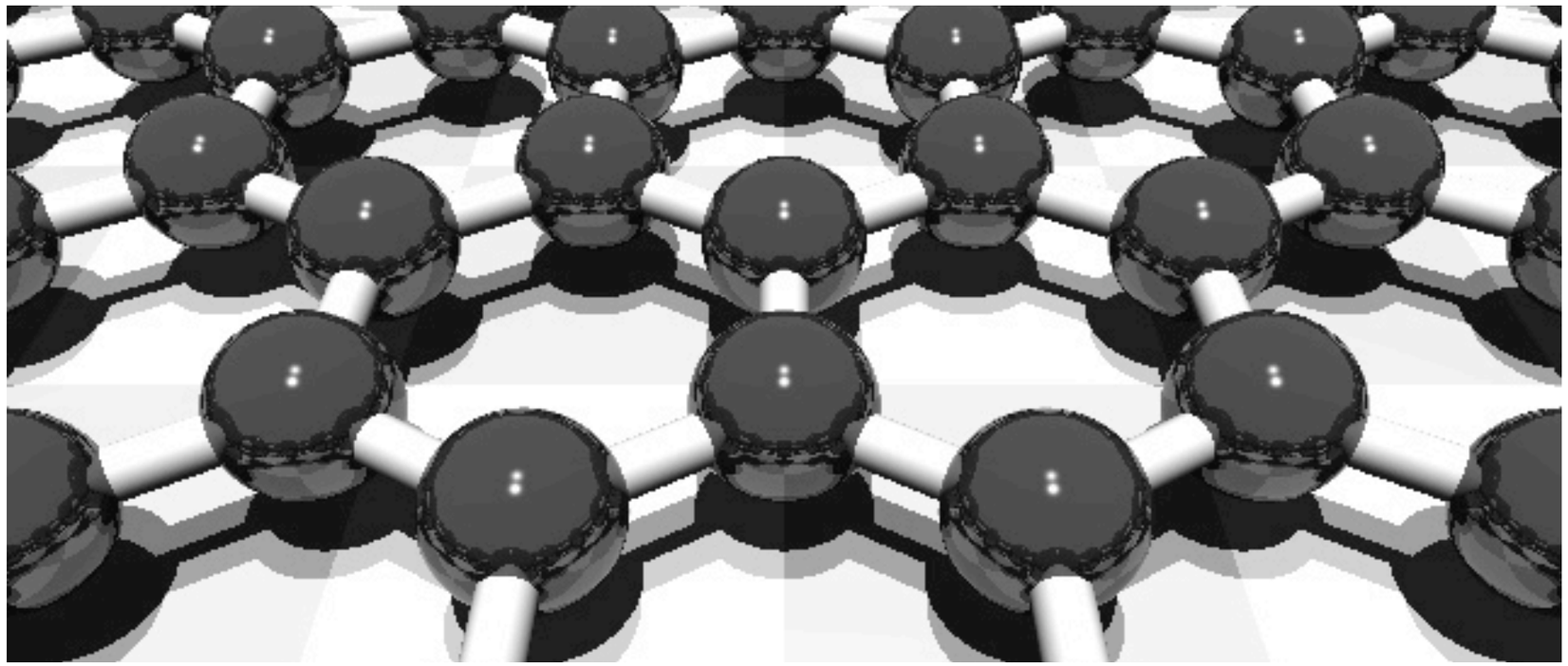
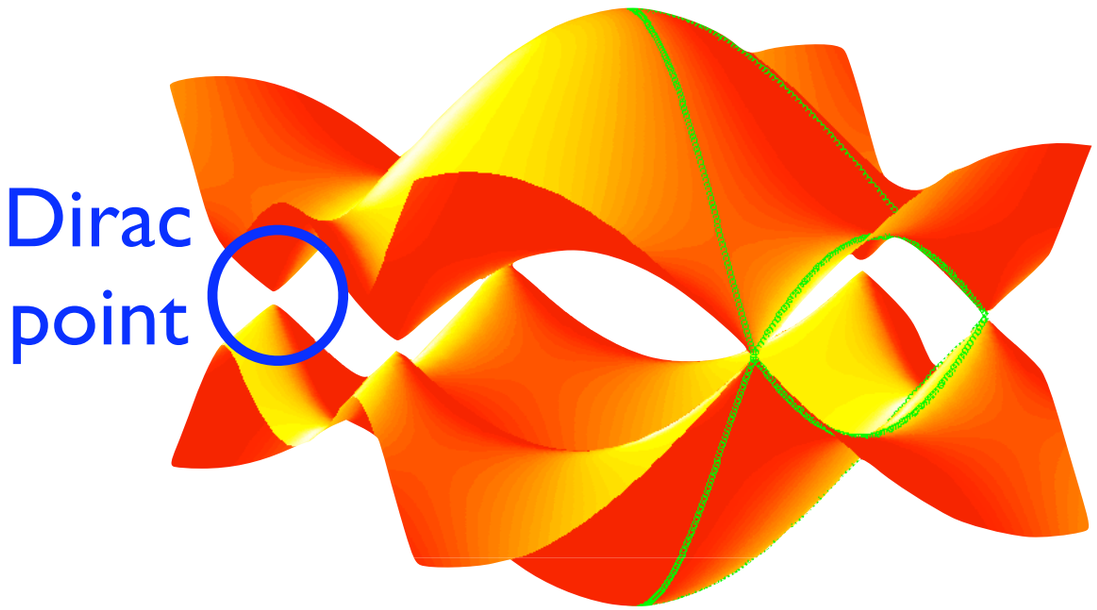
Outline

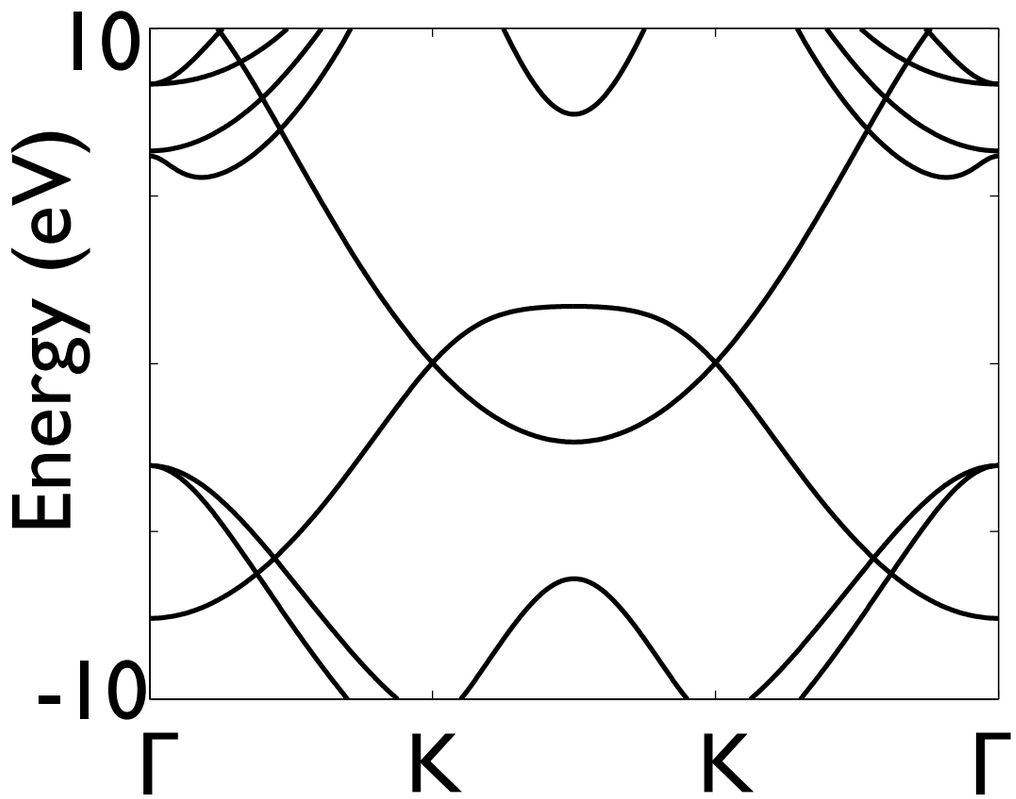
- Graphene on SiO2
- Hydrogenated graphene on SiO2
- Electron transport with FHI-aims



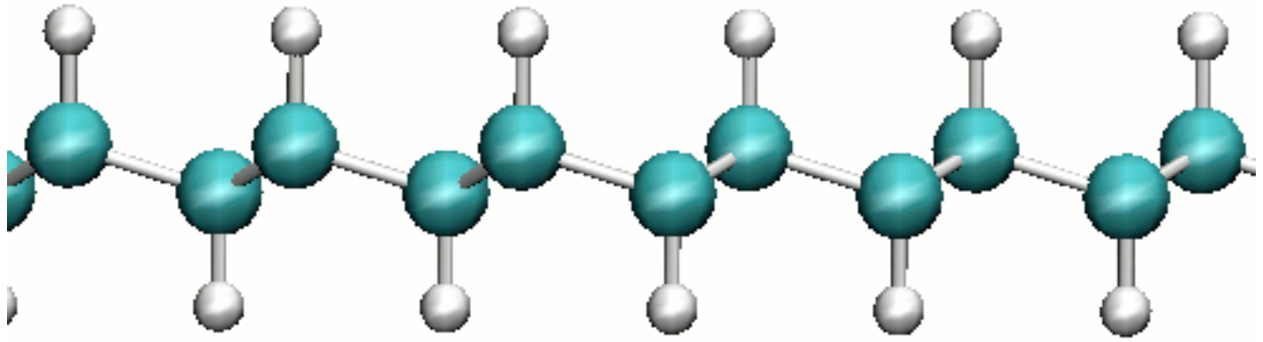
Graphene: 2D Carbon

- Perfect semi-metal with linear dispersion
- Carbon atomic configuration $(1s)^2(2s)^2(2p)^2$
- Graphene: sp^2 from 2s and two p-orbitals, pz remains

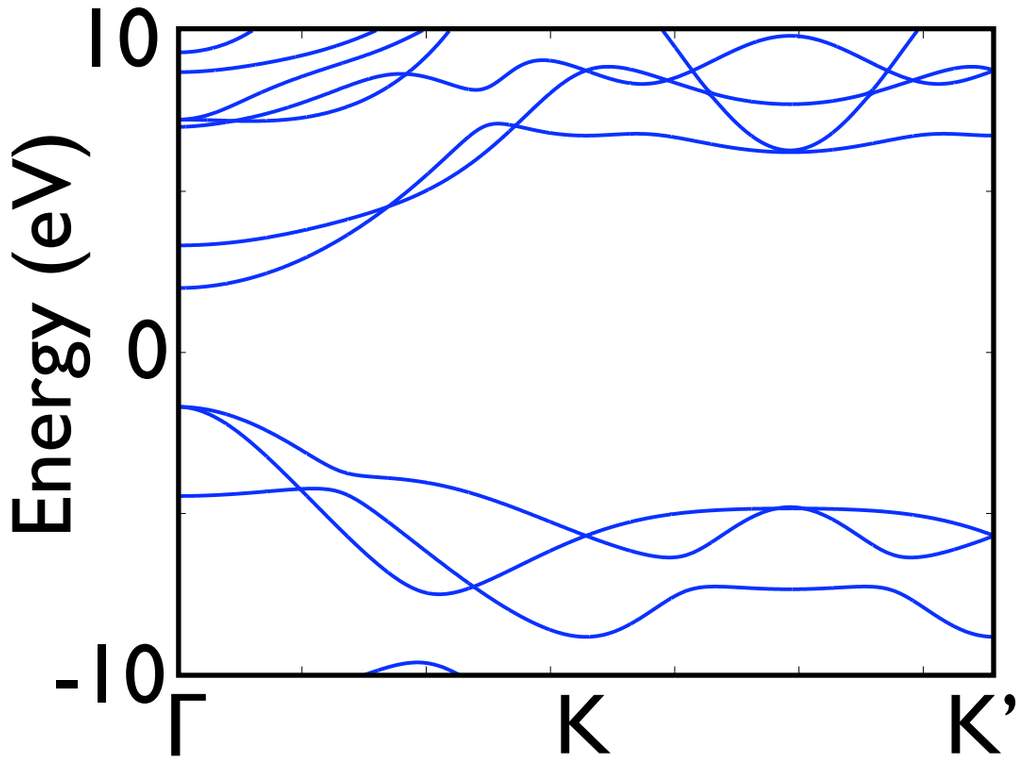




Hydrogenated graphene - Graphane



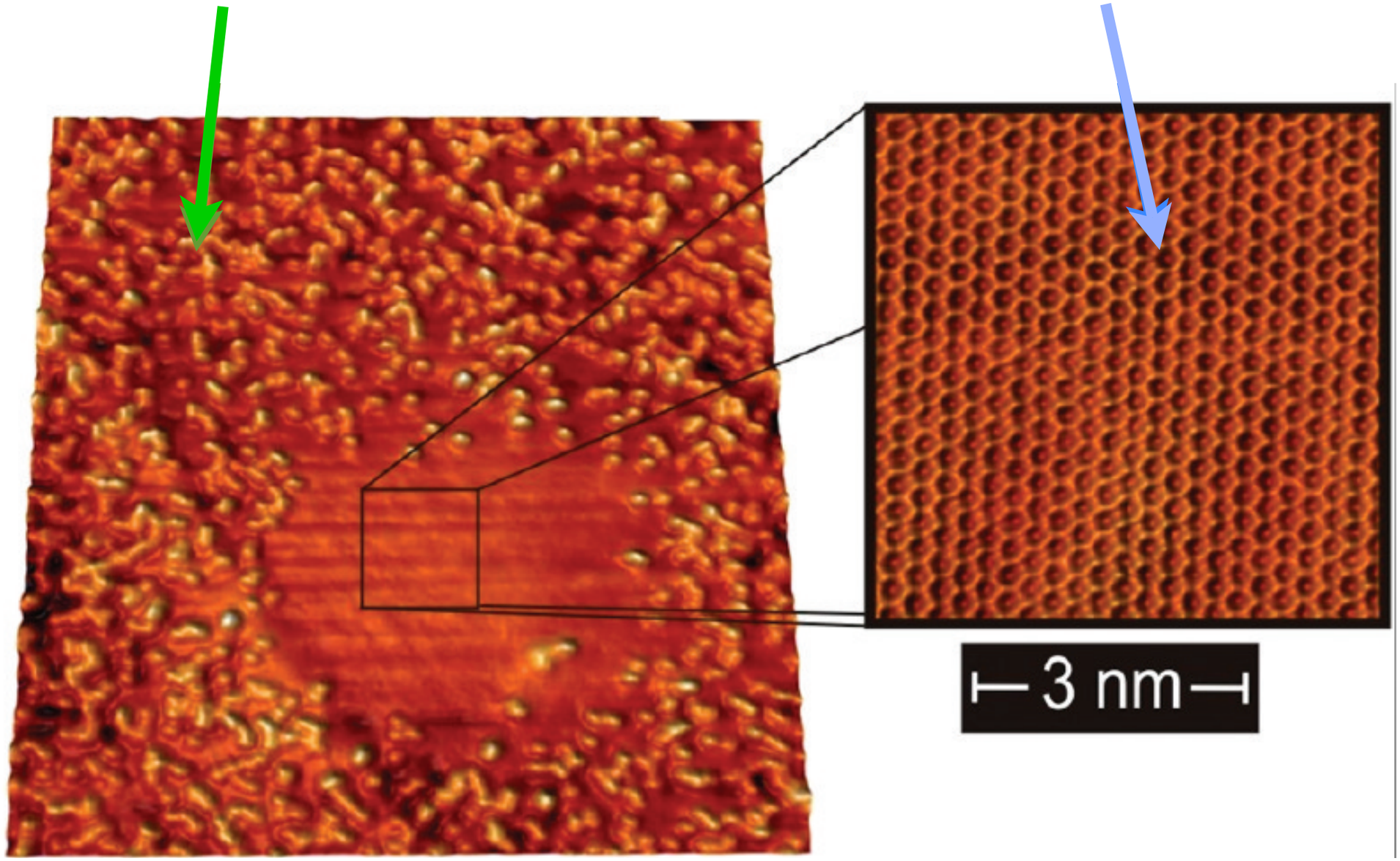
- Free-standing graphene hydrogenated on both sides is stable.
- Free-standing graphene hydrogenated only on single side is not theoretically stable.
- Graphane is an insulator



Hydrogenated graphene in experiments

- Typically placed on surfaces

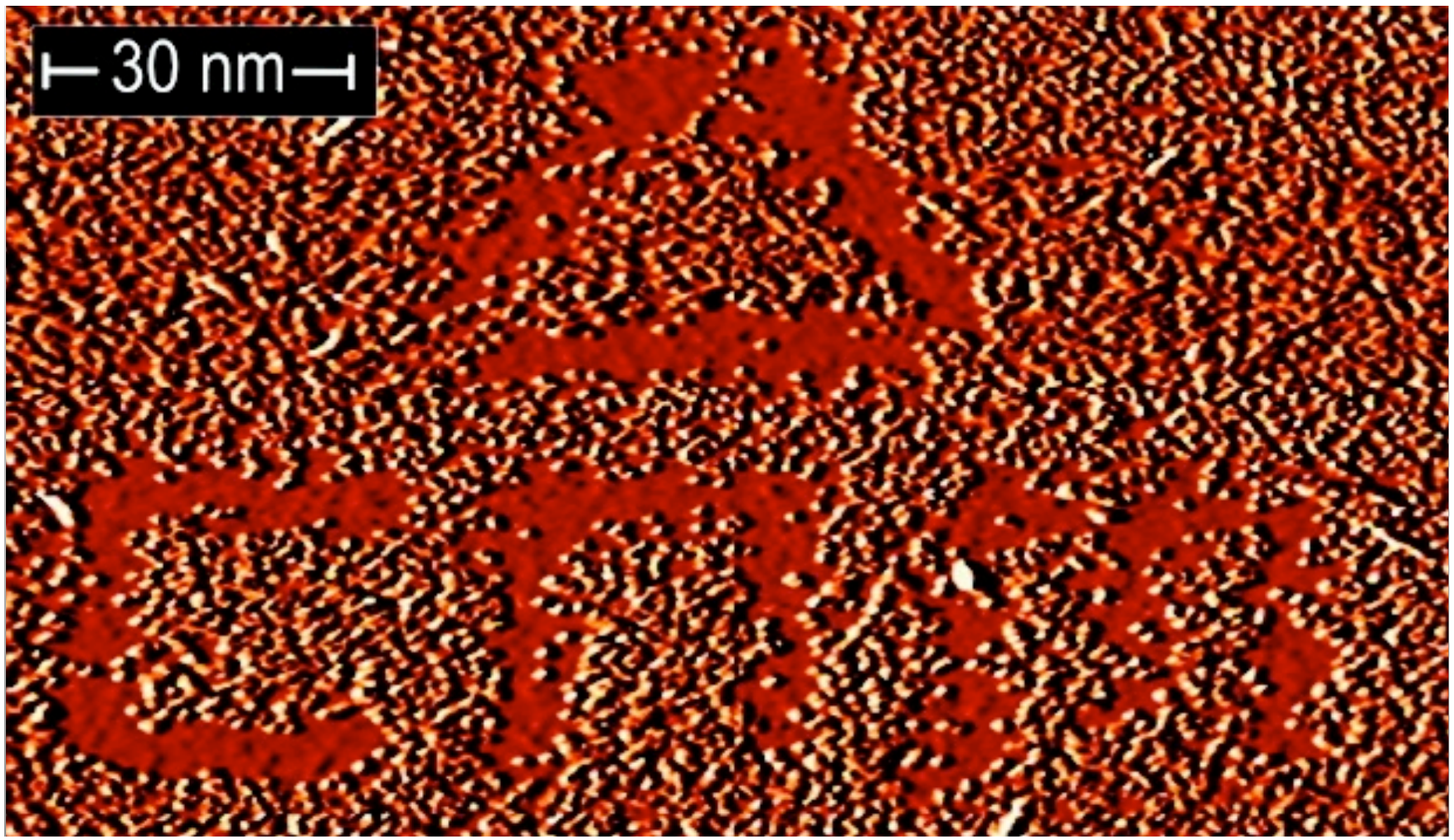
Hydrogenated graphene and hydrogens removed by STM.



Paolo Sessi et al., Nano Lett, **9**, 4343 (2009).

Hydrogenated graphene in experiments

- Writable graphene circuit board?

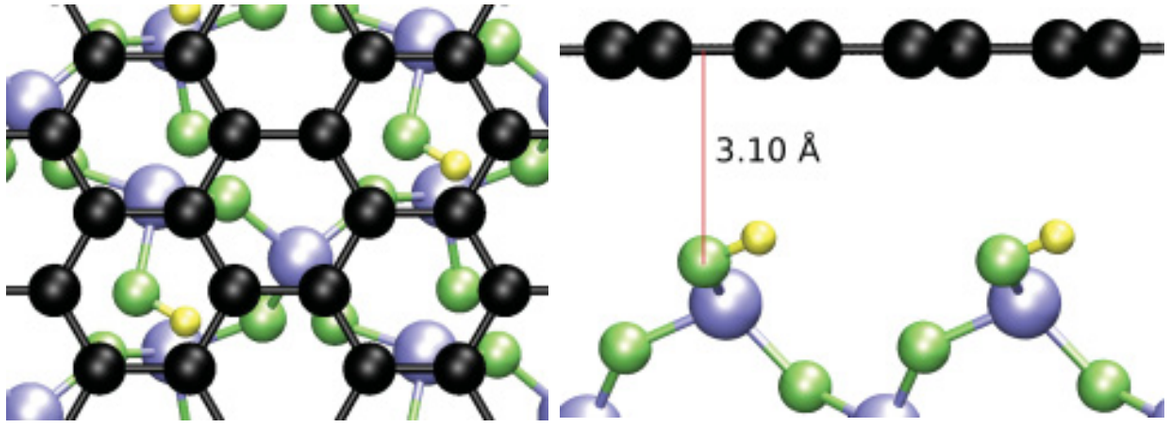


Paolo Sessi et al., Nano Lett, 9, 4343 (2009)

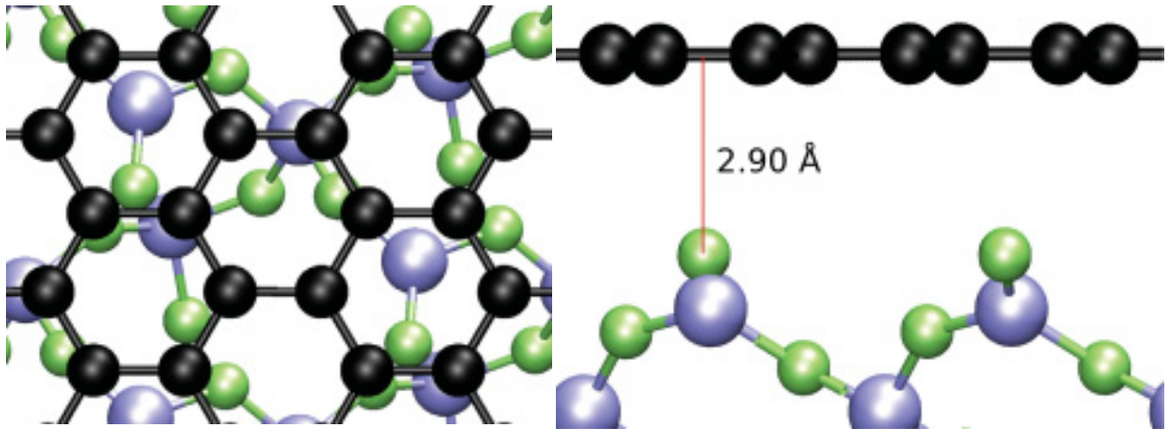
Graphene on SiO2

- In our study we use 4 different surfaces

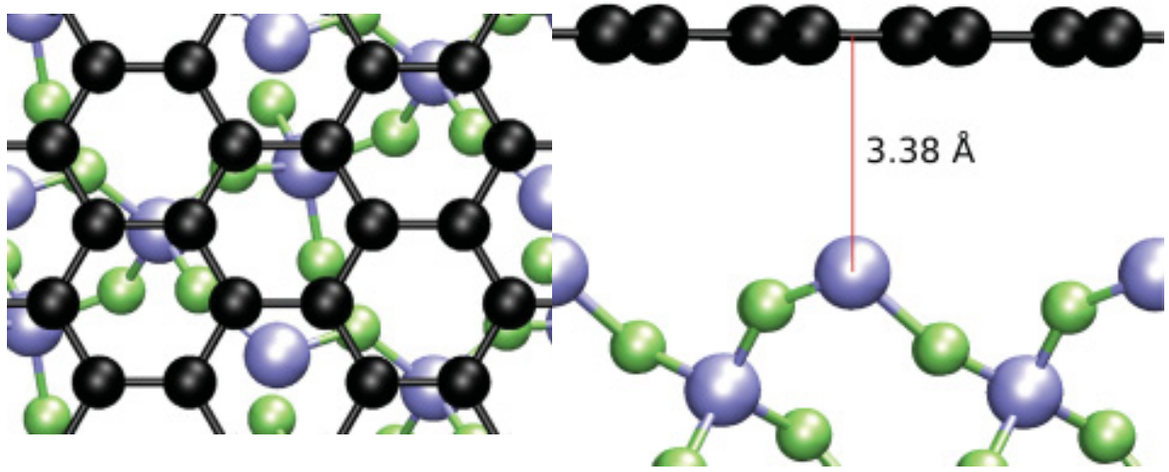
OH Terminated



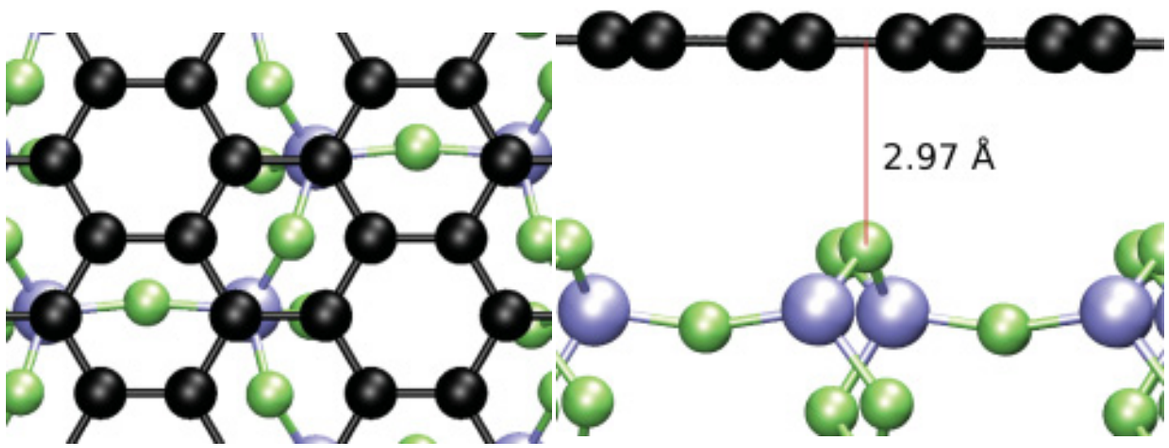
O Terminated



Si Terminated



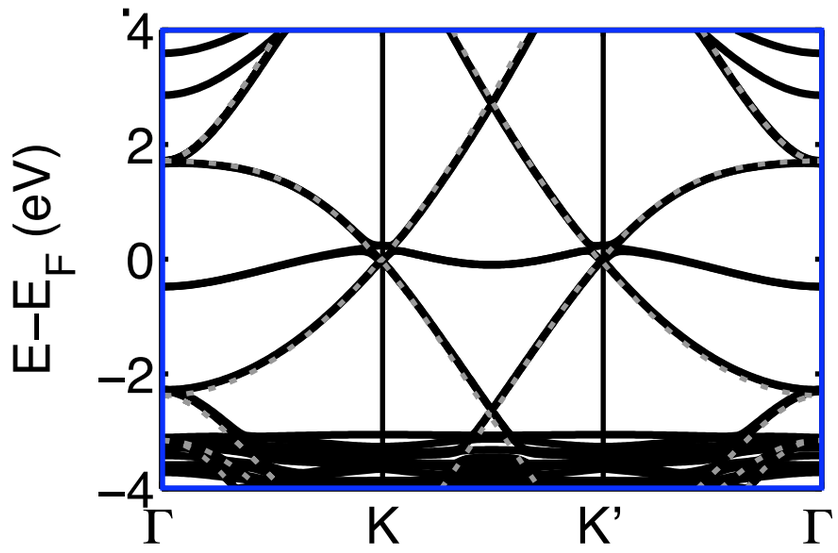
Reconstructed O Terminated



Graphene on SiO2

- Bands are close to isolated graphene

OH Terminated



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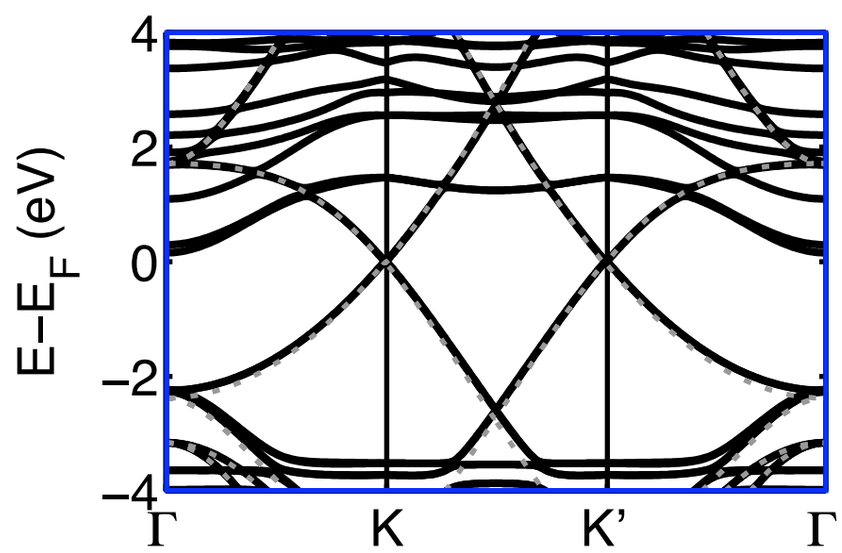
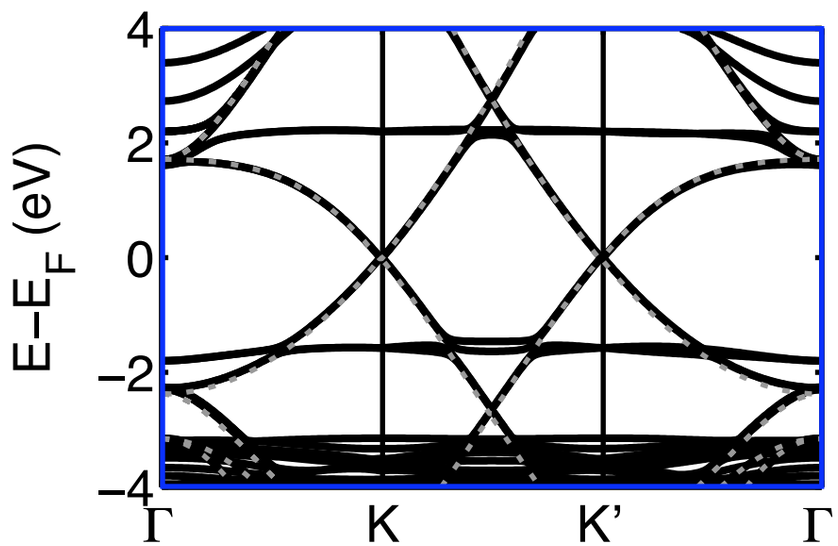
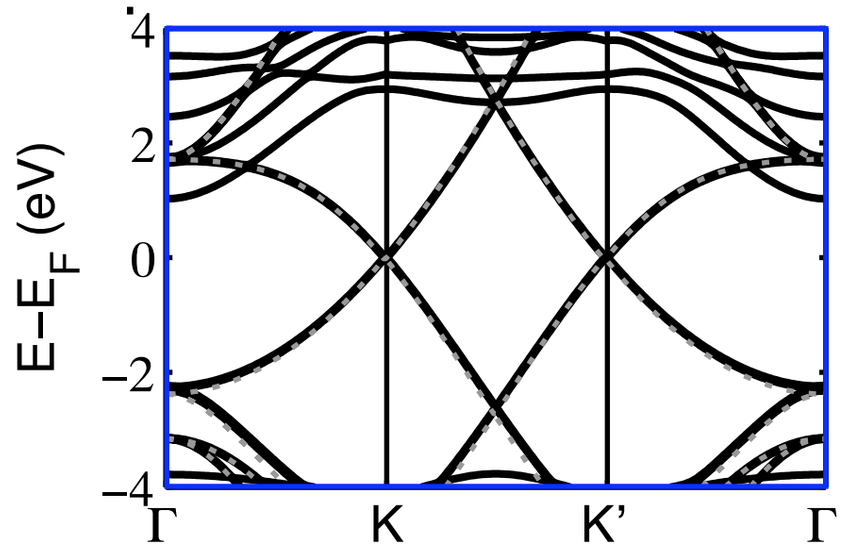


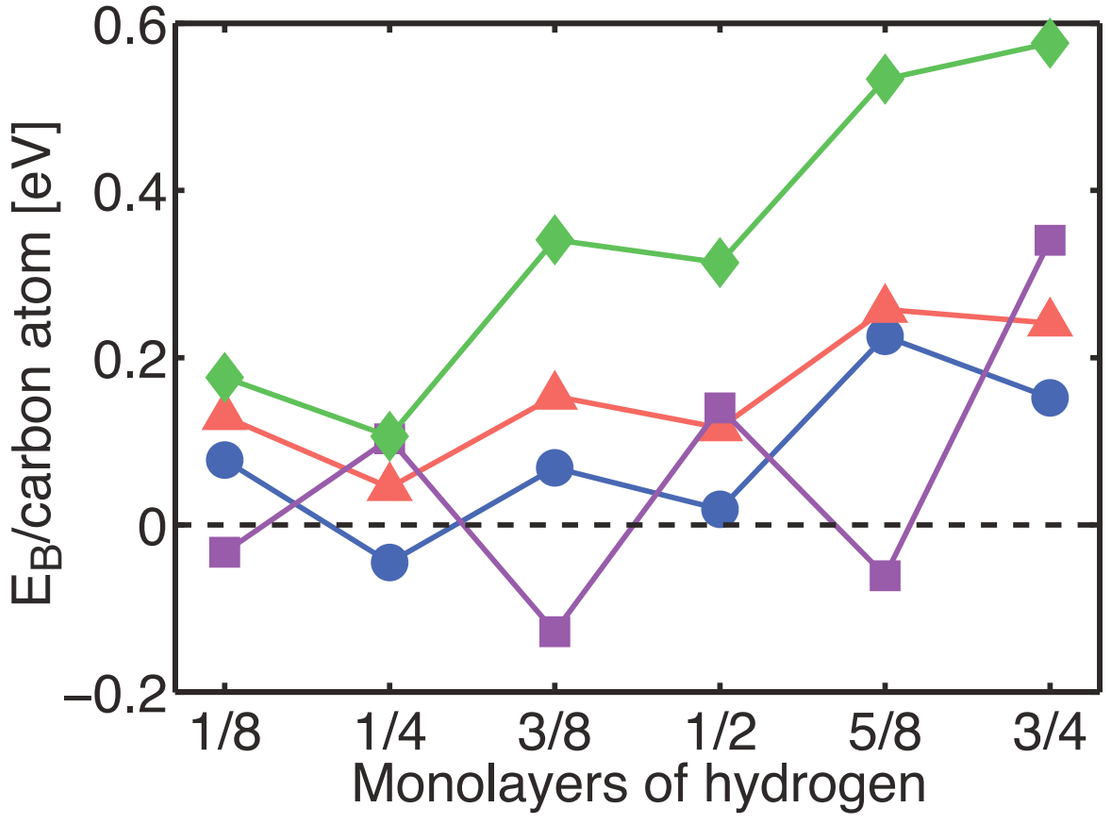
Si Terminated

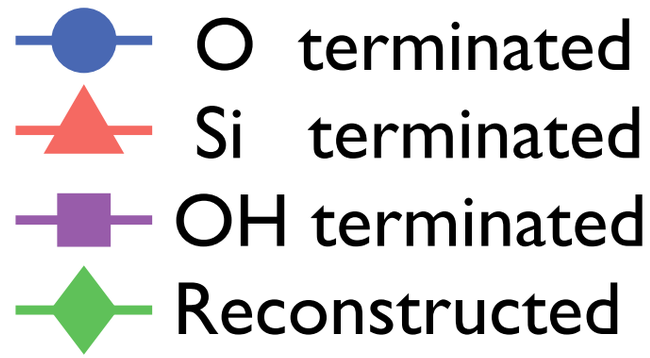


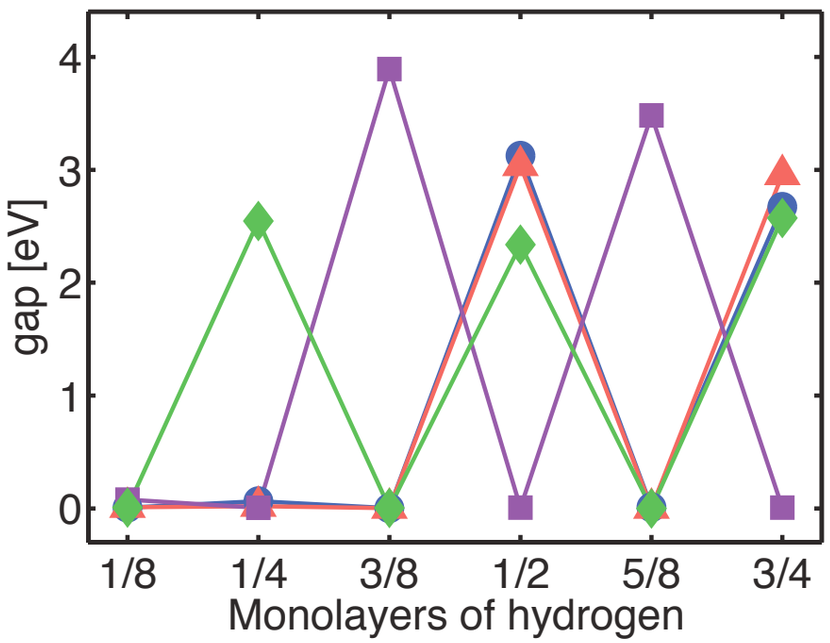
Reconstructed

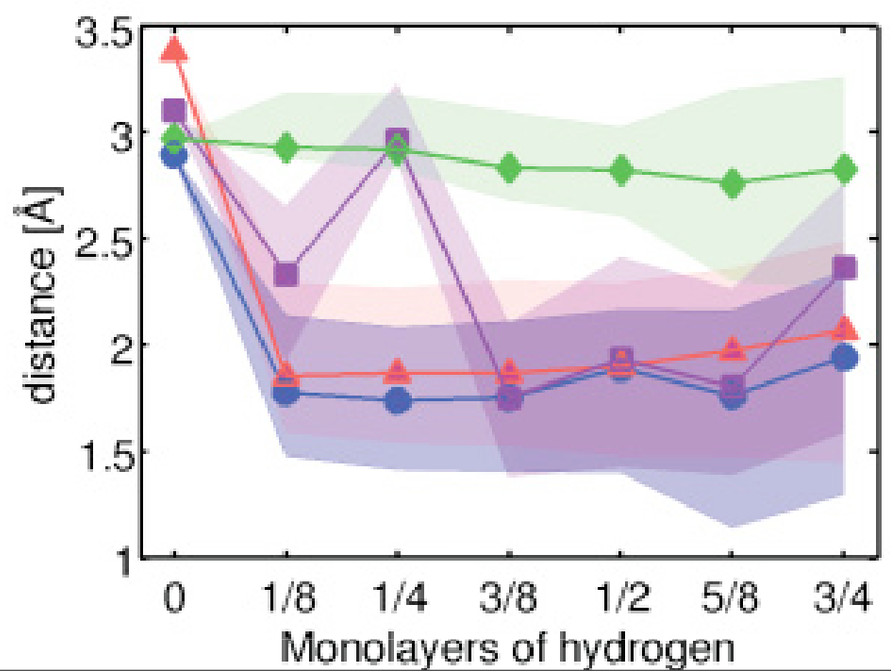


Graphane on SiO2



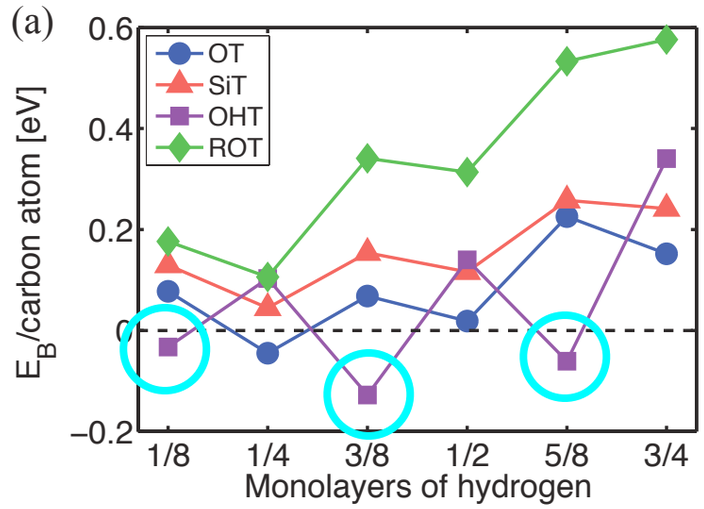


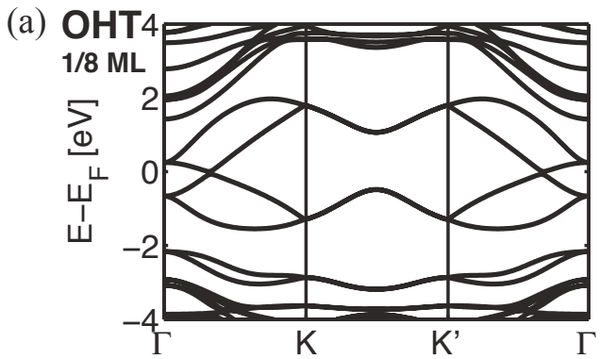


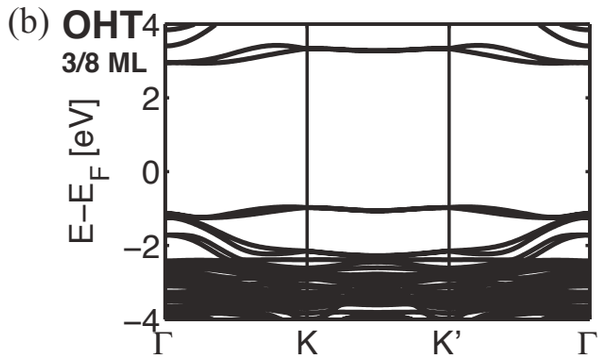


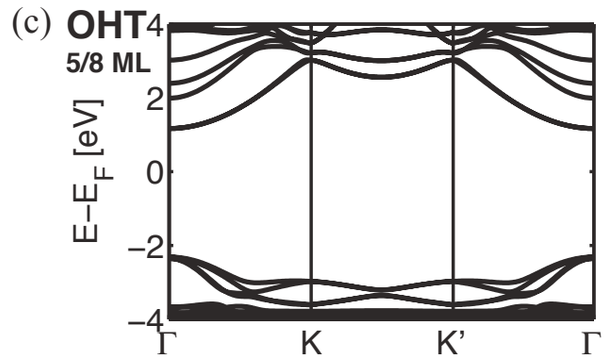
Graphane on SiO2 - OH terminated surface

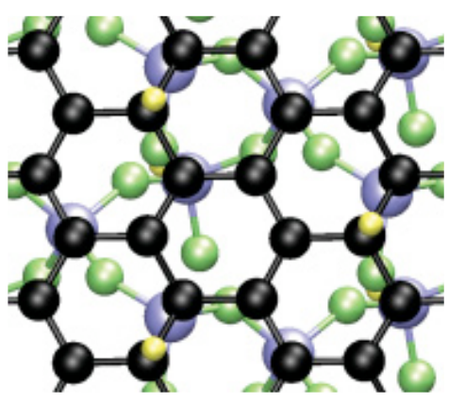
- 3 stable geometries with OH terminated surface.

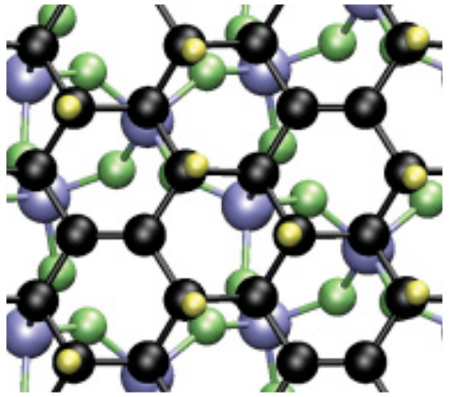


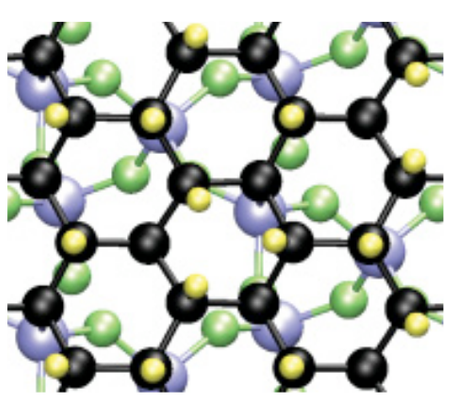


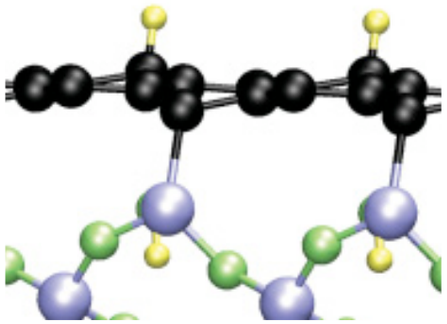


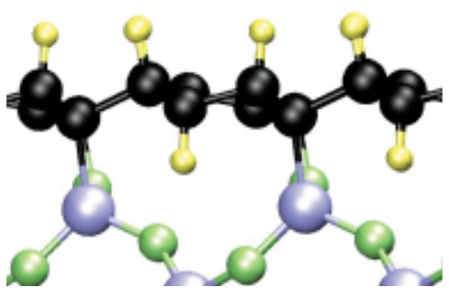


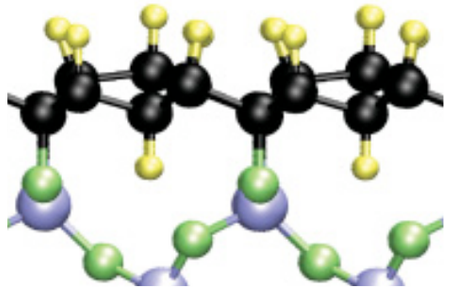






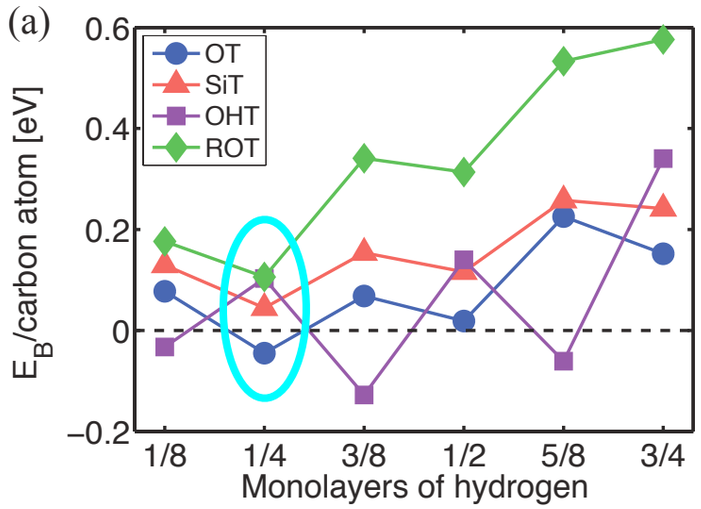


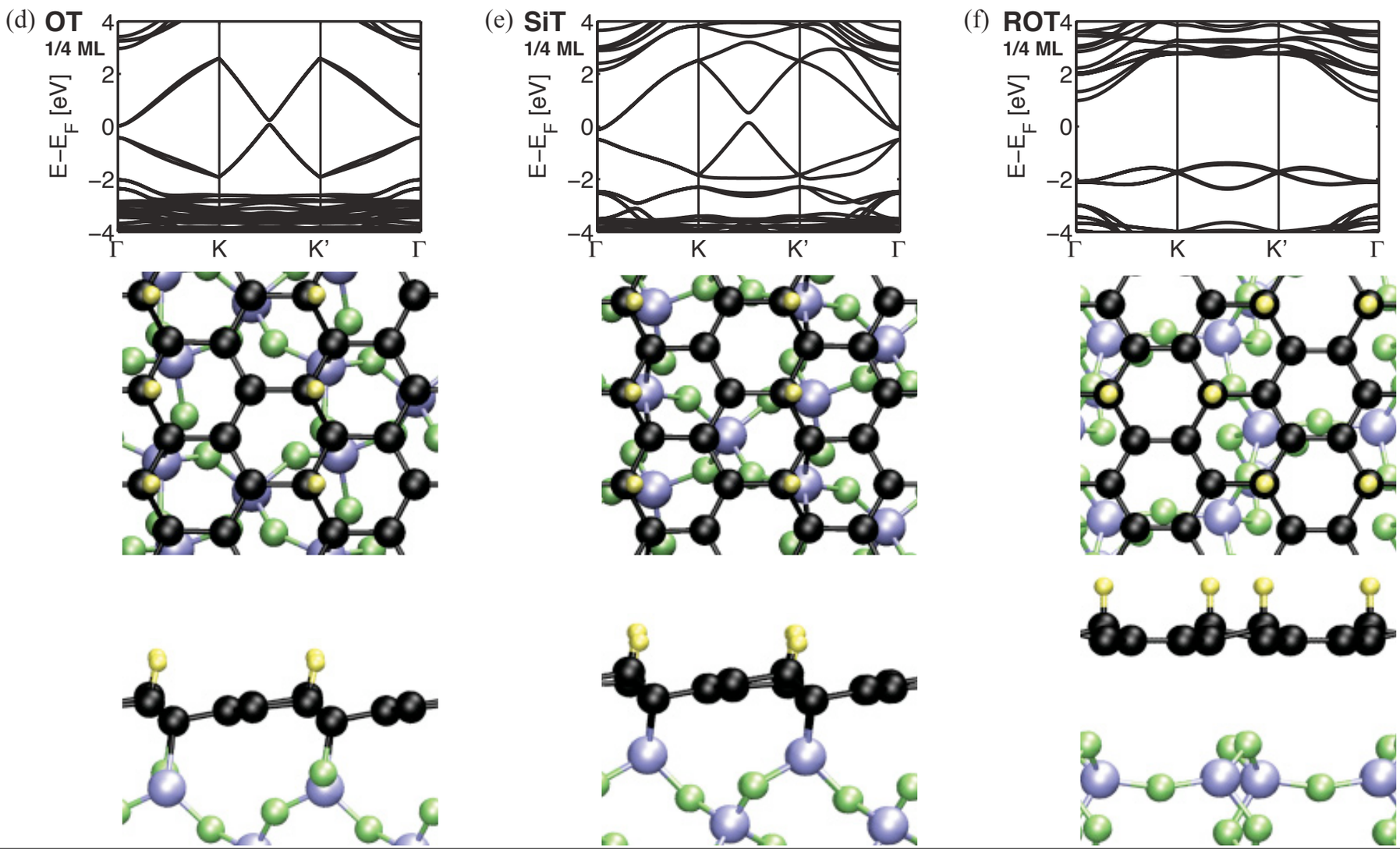




Graphane on SiO2

- O, Si and reconstructed surfaces are most stable at 1/4 filling of H.

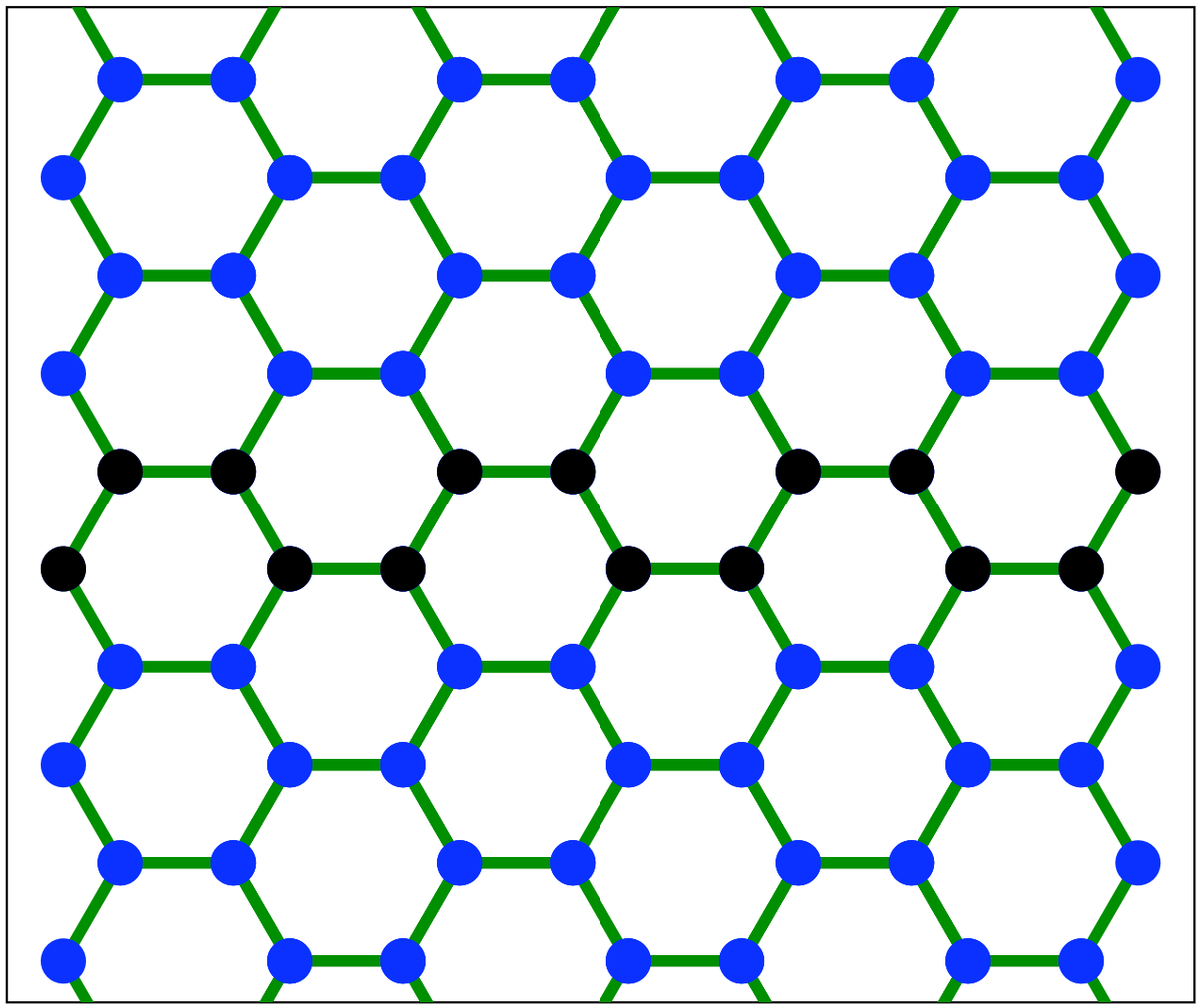




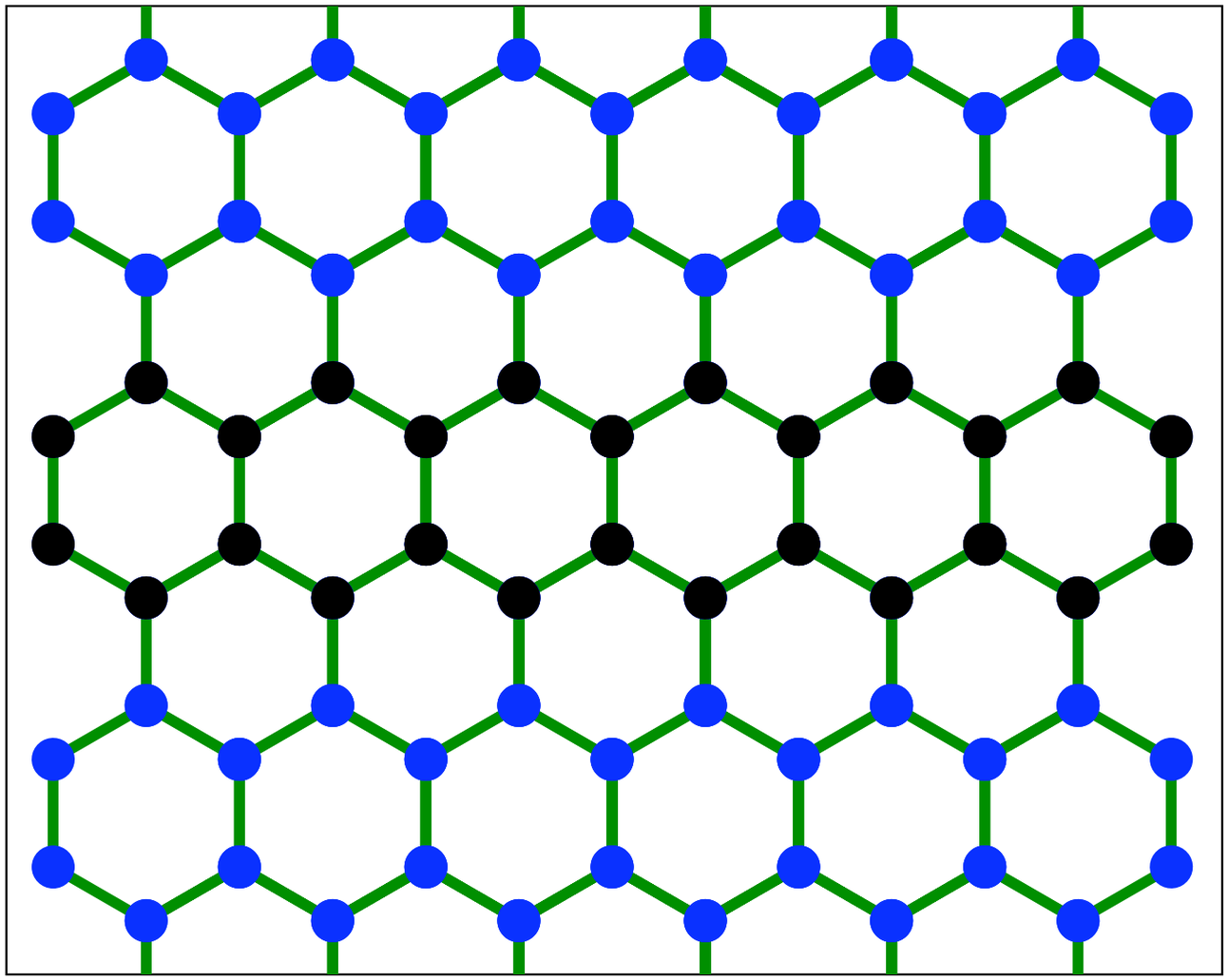
Graphene nanoribbons

Two basic types:

Armchair



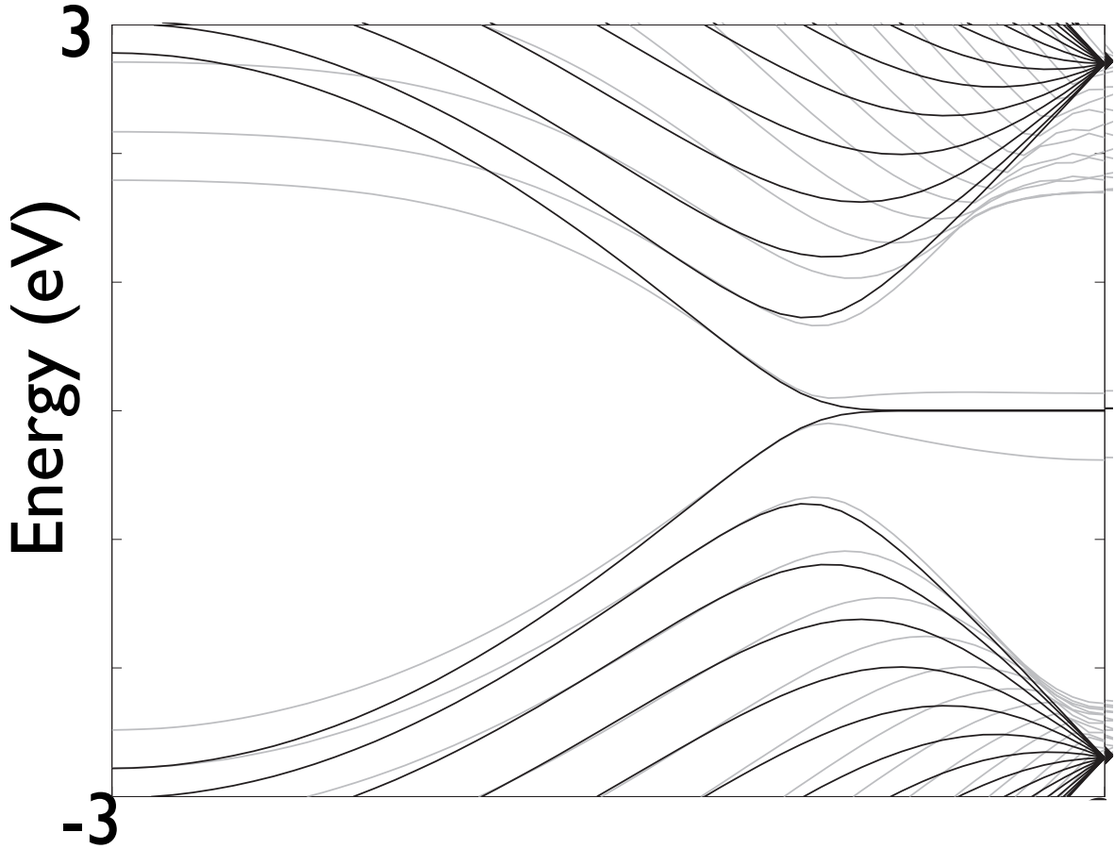
Zigzag



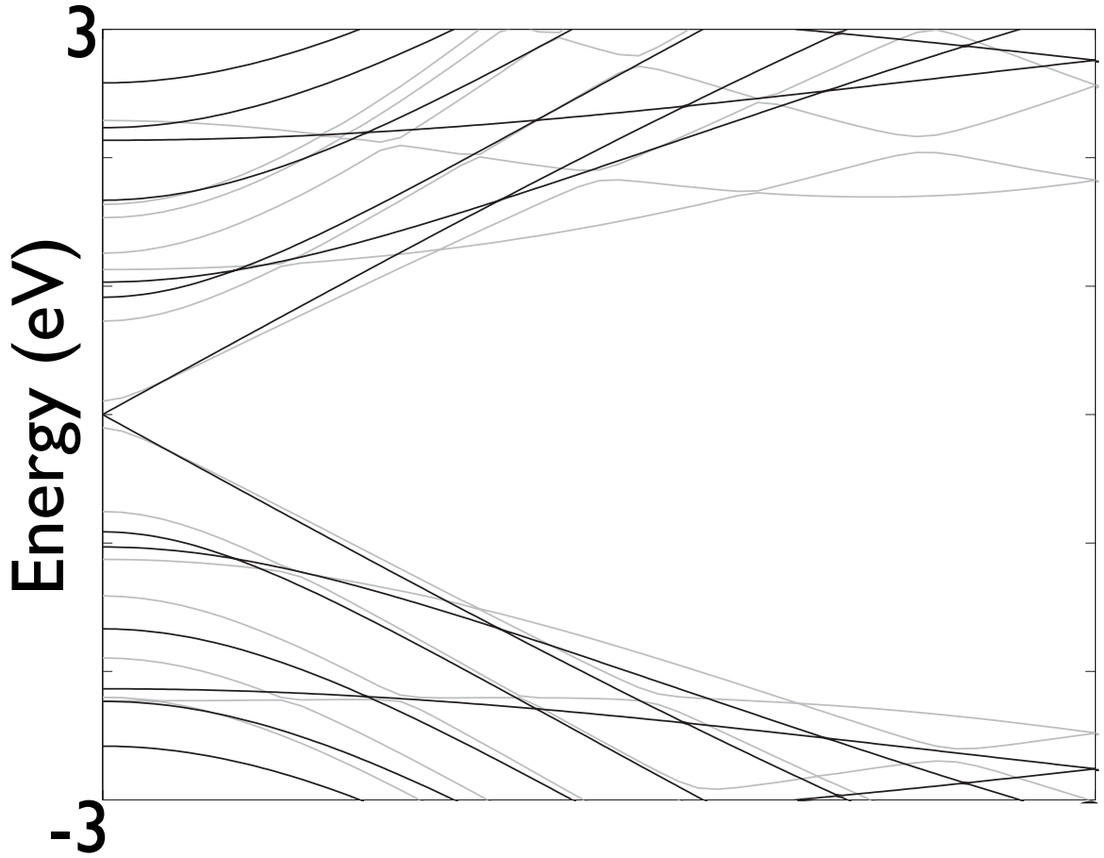
Graphene nanoribbons

Different electronic structures:

Zigzag



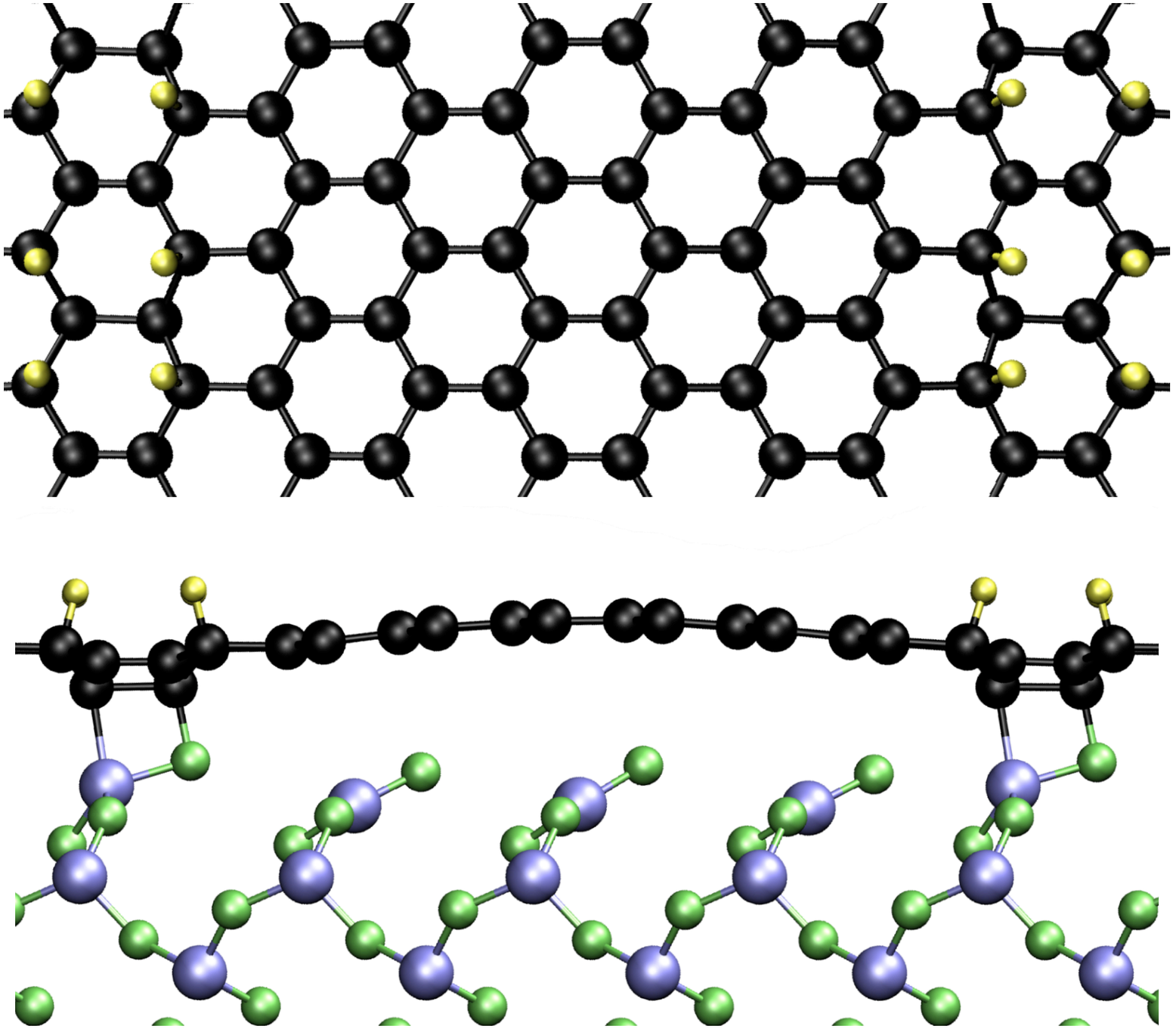
Armchair



Simple Tight-binding and Density-functional theory

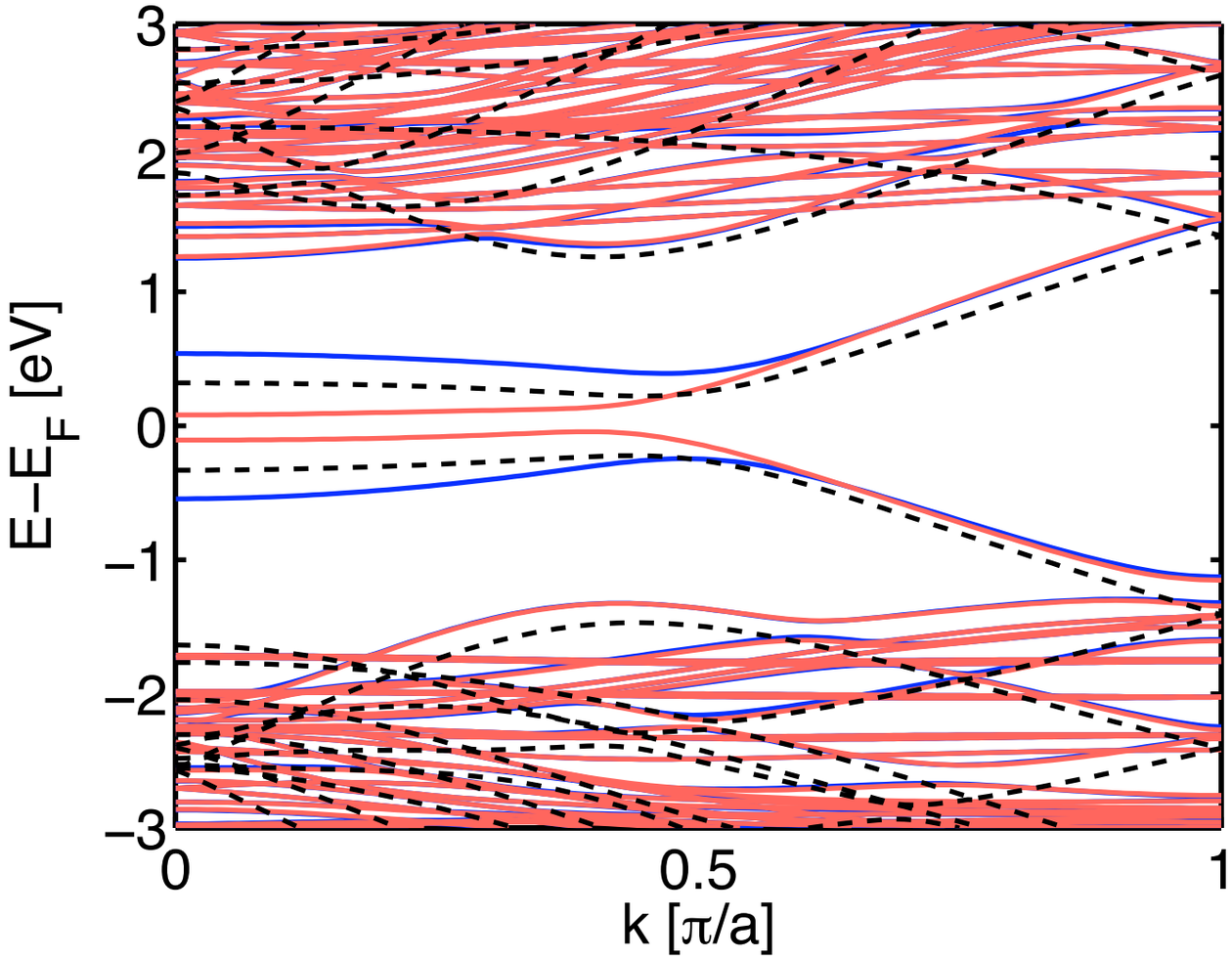
Edge magnetism:
longer range hopping and
interaction needed

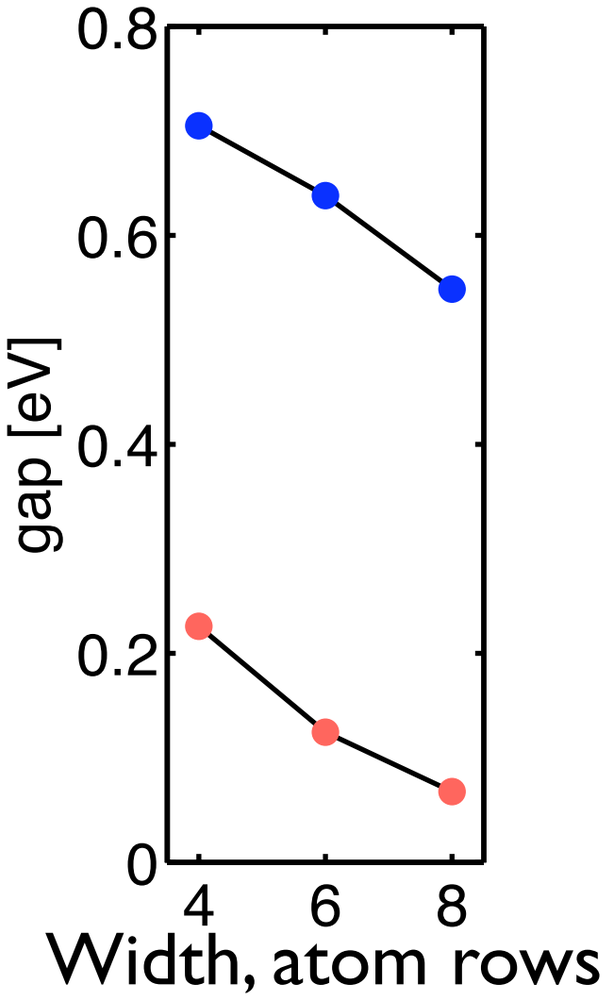
Graphane nanoribbons on SiO2

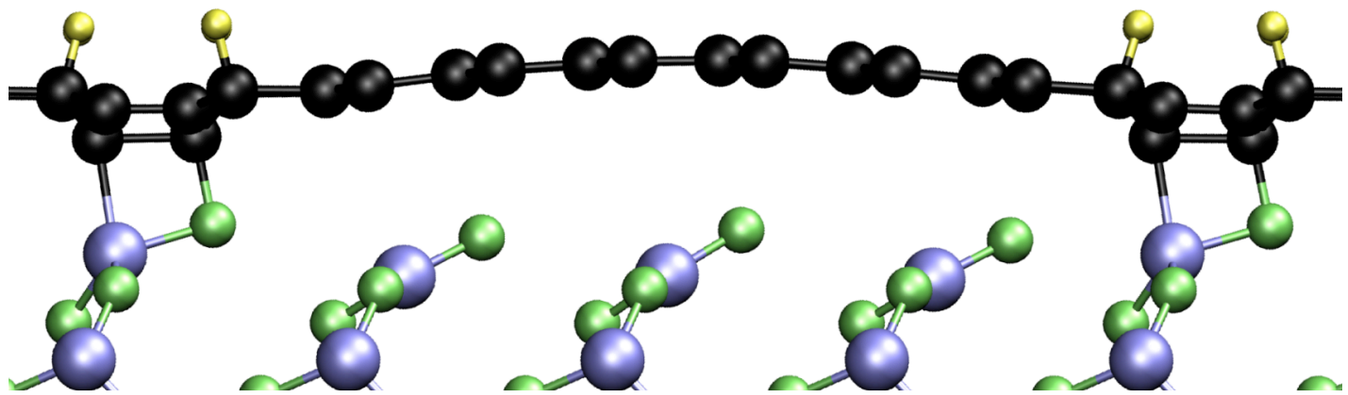


Electronic structure

- Spin-dependent bands (up and down)







Summary of graphene

- The substrate has a big effect on the properties of one side hydrogenated graphene.

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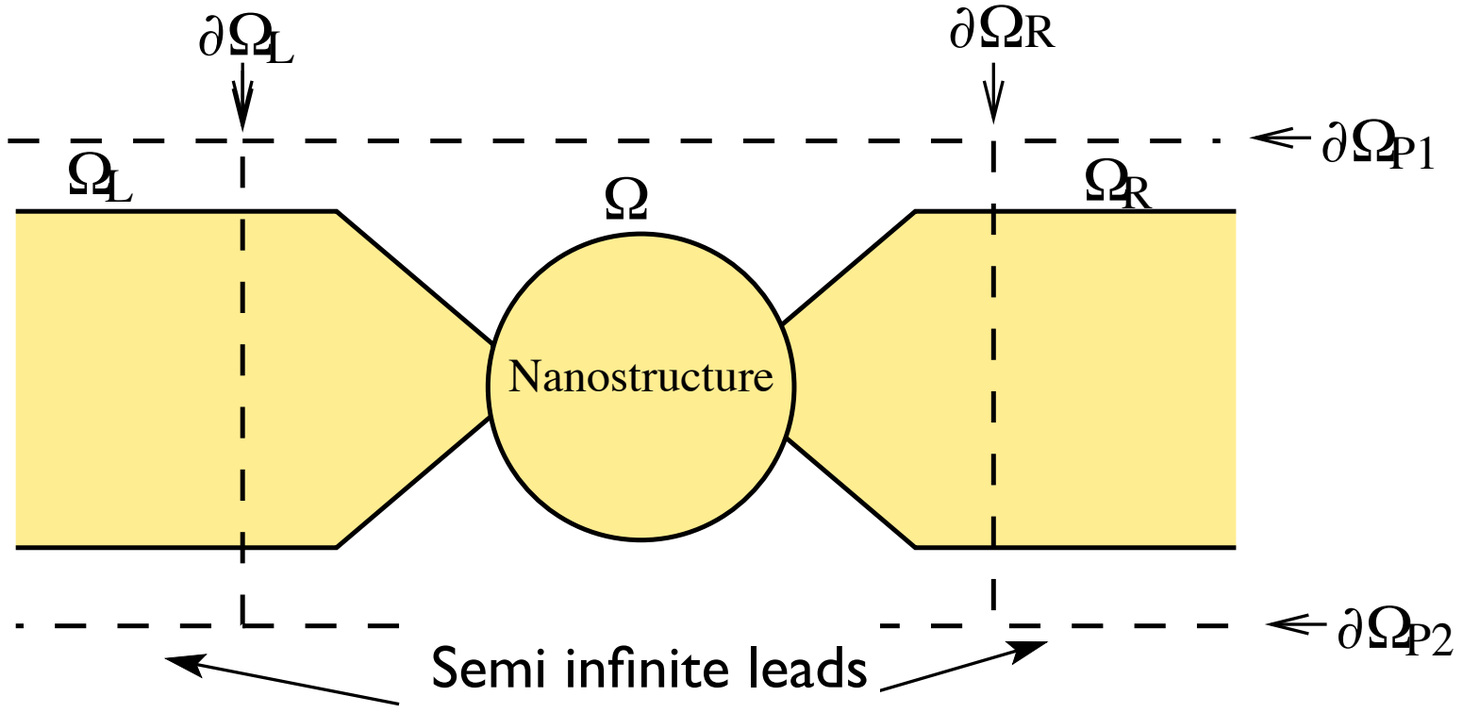
Transport in FHI-aims



- Electron tunneling through the nano structure with semi-infinite leads
- Zero-bias transport limit
- Use of gate voltage possible (adding or removing electrons)

$$T(\omega) = \int_{\partial\Omega_L}\int_{\partial\Omega_L}\int_{\partial\Omega_R}\int_{\partial\Omega_R} \Gamma_L(r_L, r'_L;\omega) G^r(r'_L, r_R;\omega) \times \Gamma_R(r_R, r'_R;\omega) G^{r*}(r'_R, r_L;\omega)\, dr_L\, dr'_L\, dr_R\, dr'_R,$$

$$I = \int_{-\infty}^{\infty} T(\omega)\left(f_L(\omega) - f_R(\omega)\right) d\omega$$

Electron transport calculations with FHI-aims

- Possibility to compare to other results from FHI-aims

- Local basis functions (Important to test that there is enough.)
- Radii of the basis functions are large

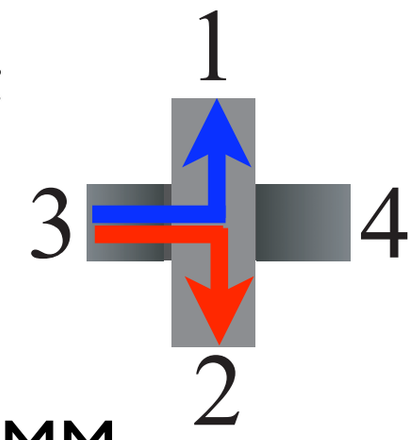
- All electron ⇒ a lot of basis functions (core states projection)

- 2-4 leads, flexible boundary conditions
- Parallelization: lapack and scalapack.
  - boundary conditions: lapack - over leads
  - center region lapack / scalapack

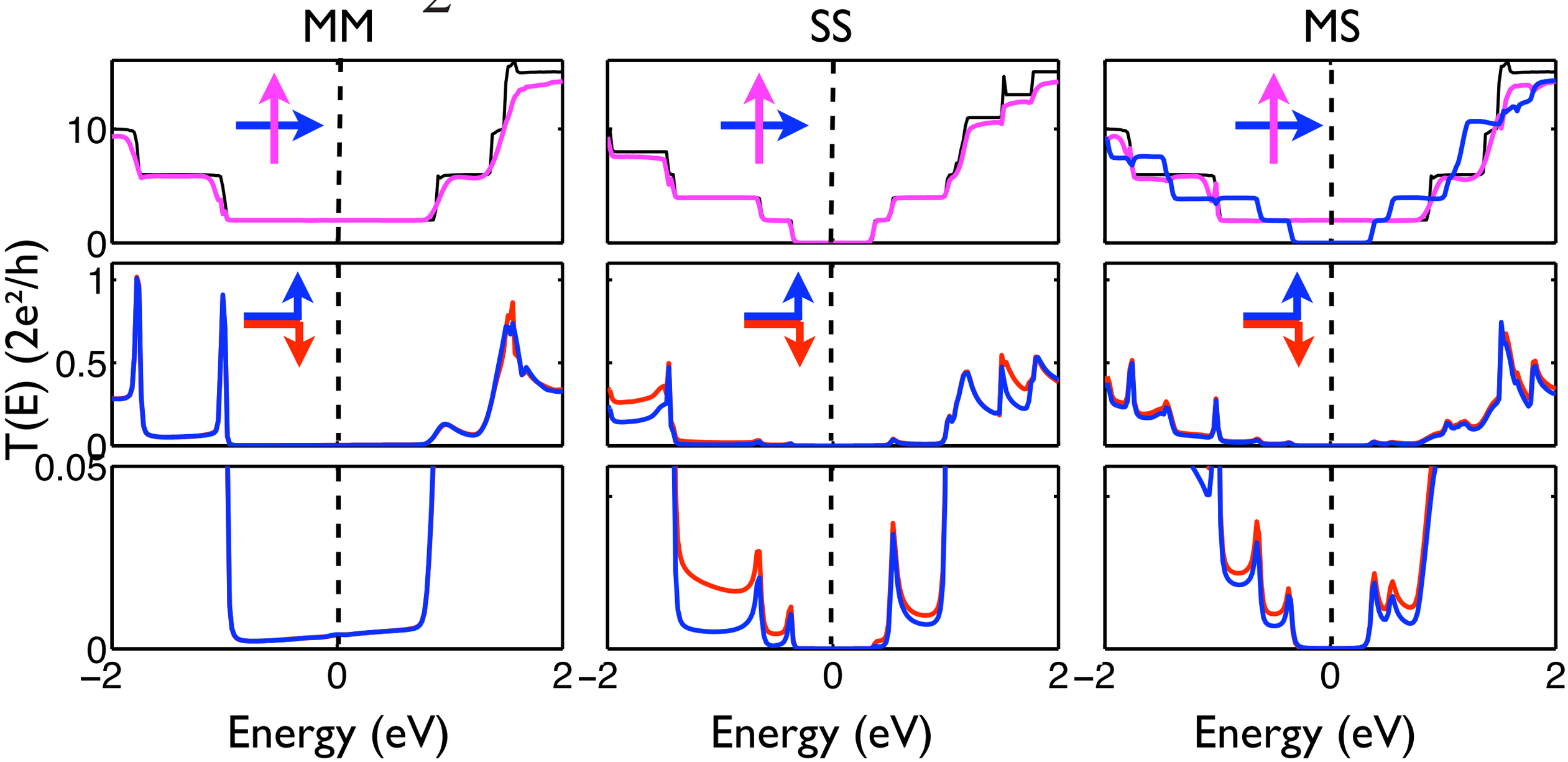
- Reference potential level is smallest eigenvalue of atoms

Example: Transport properties of junctions

Junction:

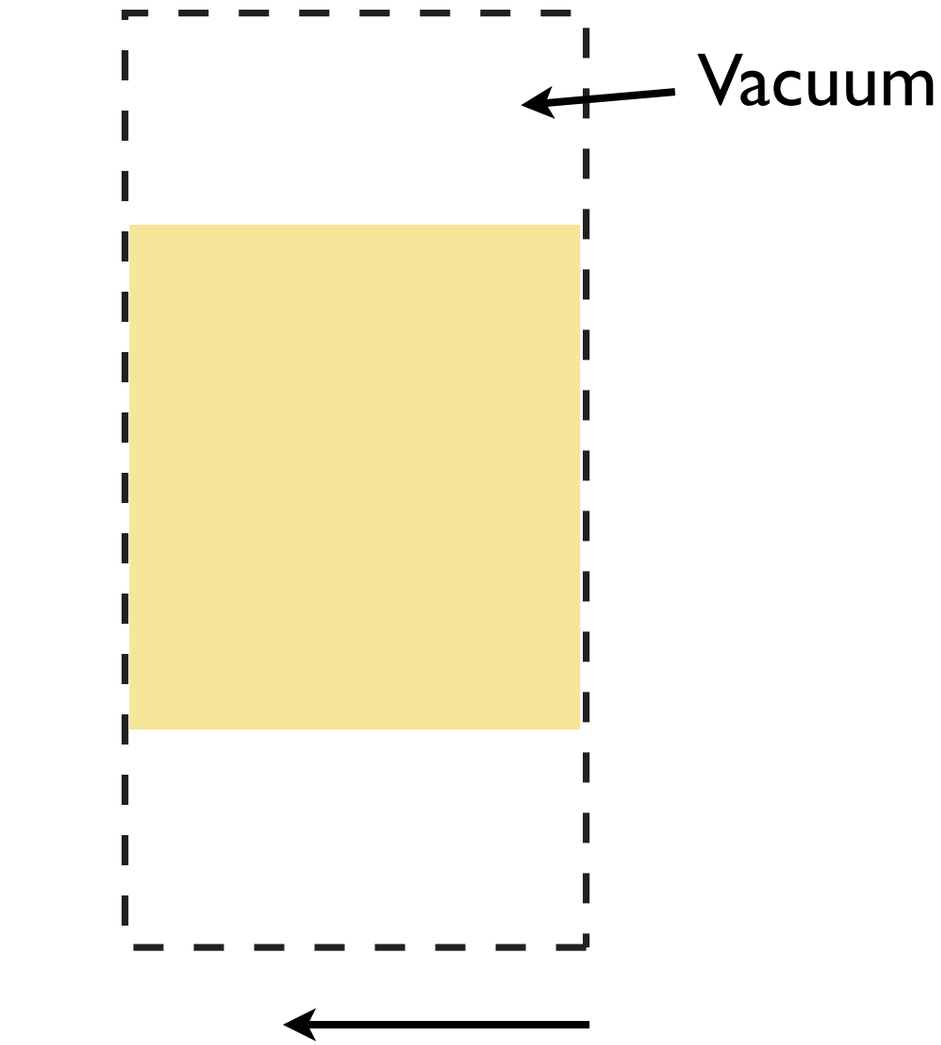


$$G = \frac{2e^2}{\pi} \int_{-\infty}^{\infty} T(E) \left(-\frac{\partial f(E)}{\partial E} \right) dE$$



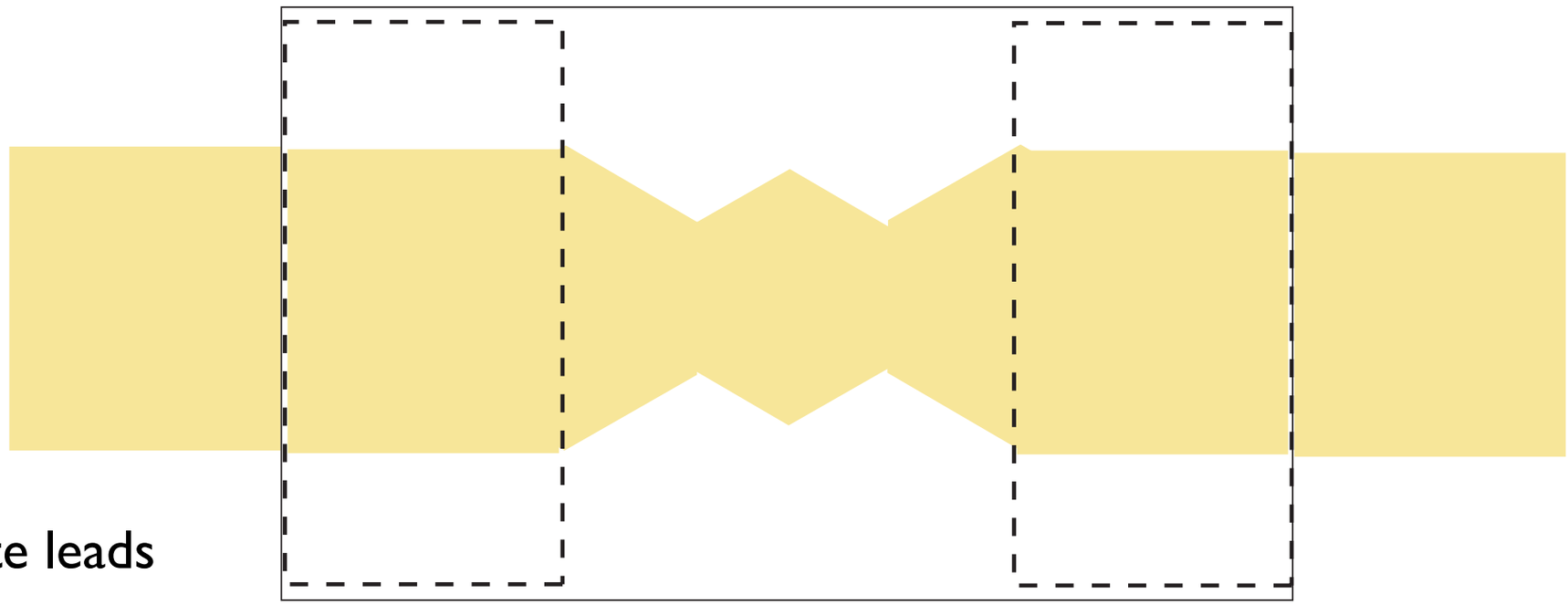
First: Semi-infinite leads

Put in to control.in: **`transport lead_calculation`**



- Lead calculation with periodic boundary conditions
- One lead calculation for each boundary
- As many k-points as it is needed (as many as in normal calculation) in transport direction
- k-points in perpendicular direction not implemented

Transport in FHI-aims

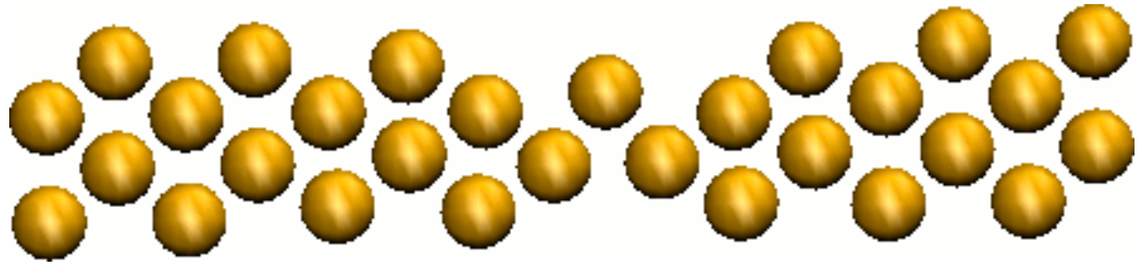


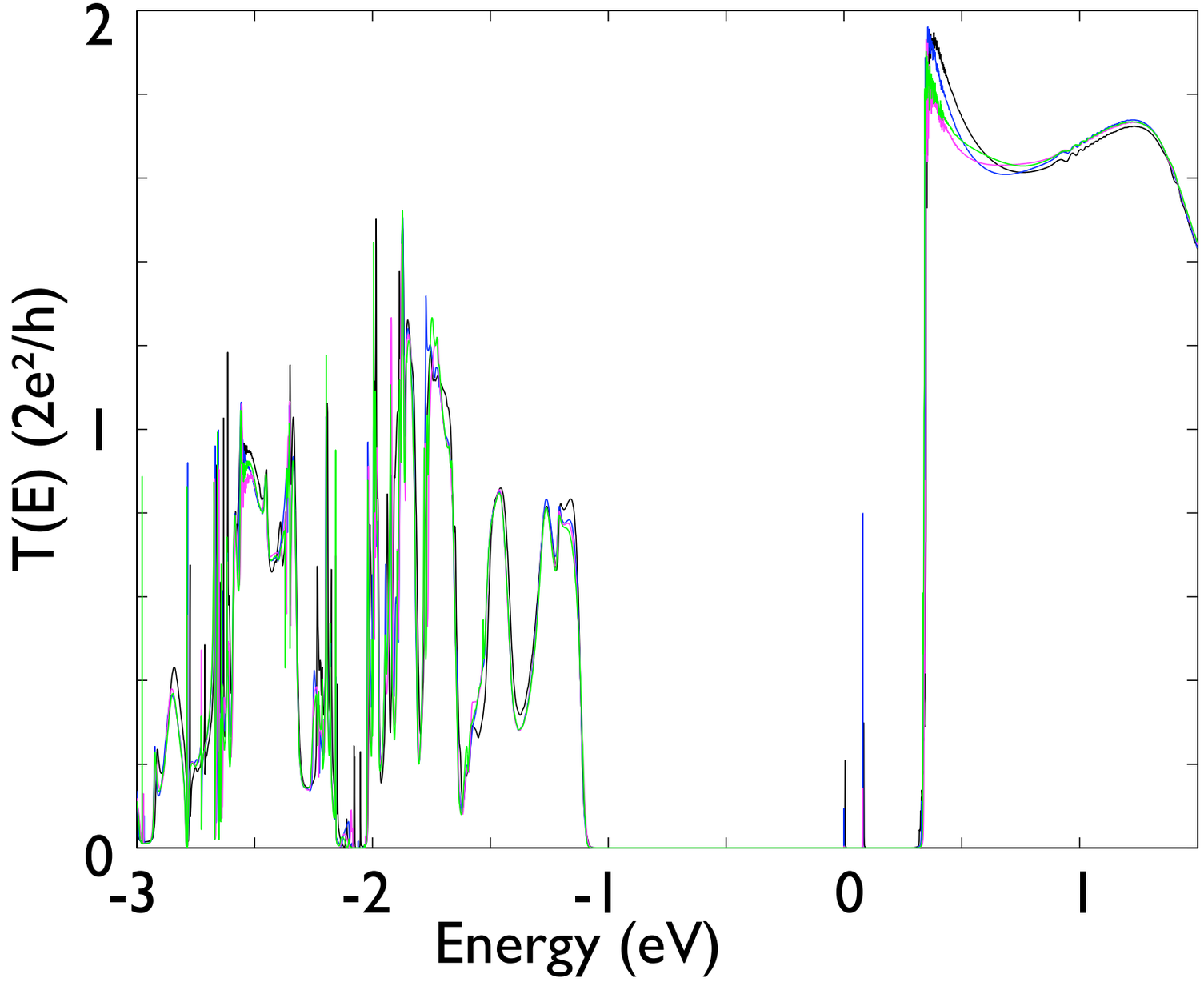
- Actual transport calculation starts with normal periodic boundary calculation.
- Parts of leads need to be in the geometry

- Computational work depends on
  - number of basis functions
  - how many basis functions are sharing leads and center region
- Boundary conditions are iterated to every energy point, T(E) separately

Au geometry examples

- The part of lead in the geometry needs to be large enough so that the potential is close to leads potential at the boundary.





- Au geometries with different lengths:
- 33Å, 49Å, 66Å and 83Å

What to put in control.in in order to get T(E)

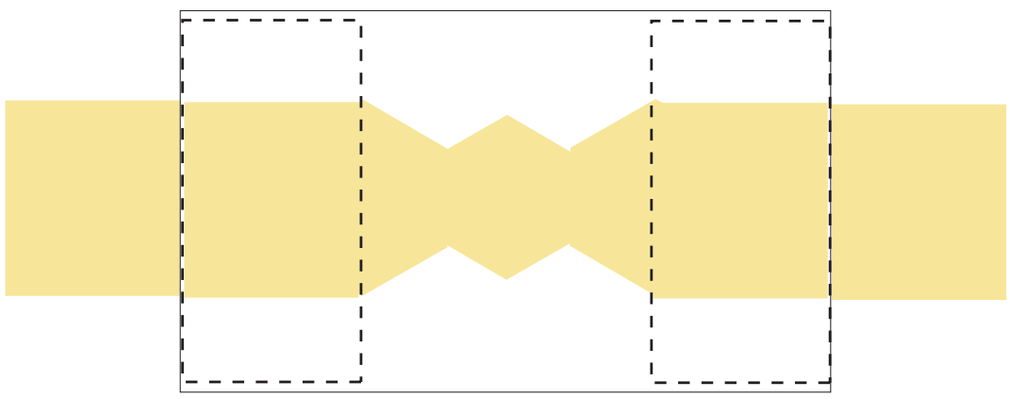
```
transport transport_calculation

transport tunneling_file_name res_file_name
transport energy_range -3.1 1.5 5000
transport lead_1 1  lead_1_file_name
transport lead_2 17 lead_2_file_name

transport number_of_boundary_iterations 100
transport boundary_treshold 0.5
transport epsilon_end       0.0001
transport epsilon_start     0.0001
transport boundary_mix      0.5
```

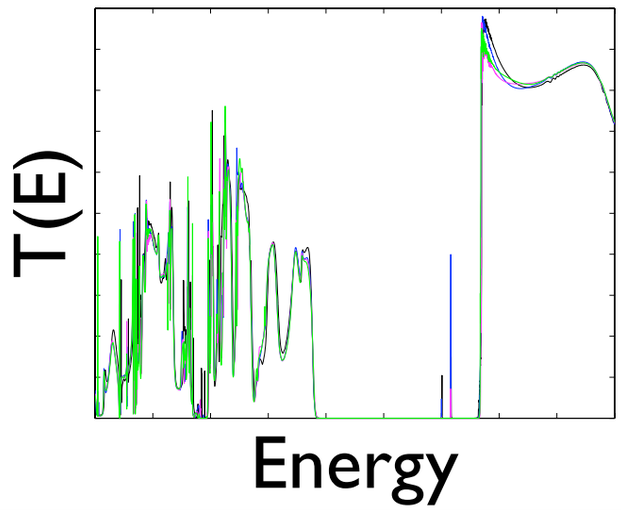
Results file:

T(E) range:

Lead definitions:

Parameters for the boundary condition iterations





Summary Transport

- Landauer-Büttiker electron transport formula is implemented in FHI-aims.

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