Functionalizing graphene by embedded boron clusters

BSW2011, Yozgat

Cem Özdoğan, Alexander Quandt, Jens Kunstmann,Holger Fehske

ozdogan@cankaya.edu.tr http://siber.cankaya.edu.tr

1 Department of Materials Science and Engineering, Çankaya University,06530 Ankara, Turkey

2 School of Physics and DST/NRF Centre of Excellence In Strong Materials, University of the Witwatersrand, Wits 2050, South Africa

3 Institute for Materials Science, TU Dresden, Hallwachstr. 3, D-01069 Dresden, Germany

4 Institut fur Physik der Universitat Greifswald, FelixHausdorff-Str. 6, D-17489 Greifswald, Germany

Introduction I

- How to scale down current silicon-based technology to the nanodomain?
- Micro Electronics $\Longrightarrow$ Nano Electronics.
- Silicon substrate + Metallic electrode
- Graphene substrate + Chains of boron clusters
- Method: Density Functional Theory.
- Exchange-correlation: Generalized Gradient Approximation (PW91).
- Basis set: Plane waves. PAW Pseudopotential.
- Code: VASP

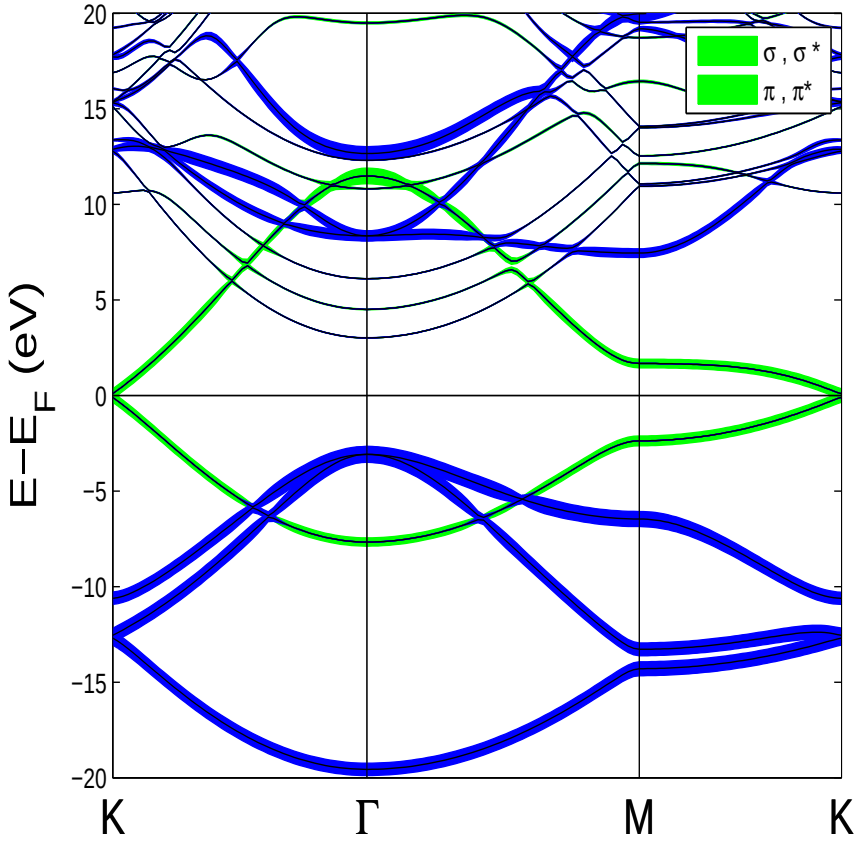
Introduction II

- Why graphene as substrate?
- A monoatamic layer is the ultimate limit for a substrate.
- Why boron clusters for wiring?
- In current silicon technology (45 nm feature size) the substrate is doped with boron clusters.
- Our suggestion: similar technique in graphite to obtain boron-functionalized graphene.

Introduction III

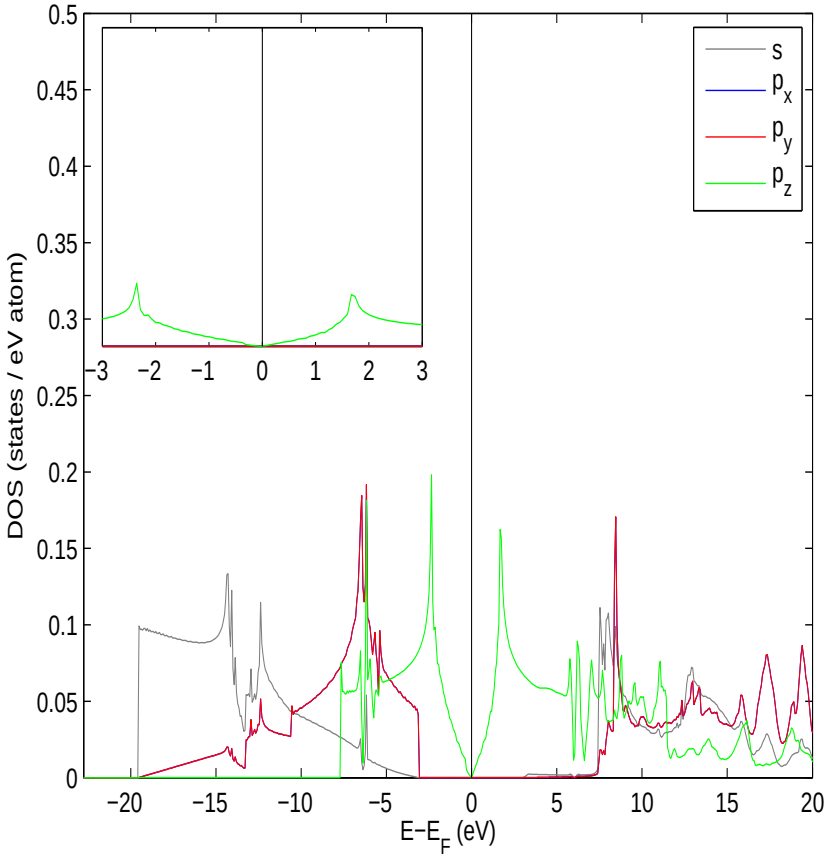
- Small boron clusters are quasiplanar and largely made from pyramidal B_7-units.
- All bulk boron nanomaterials made from these B_7-units are metallic.
- Quasiplanar boron structures are also metallic.
- Very flexible bonding and compatible bond lengths to fit into the graphene matrix.
- Boron clusters are a good building block for the metalization of graphene.

Graphene I



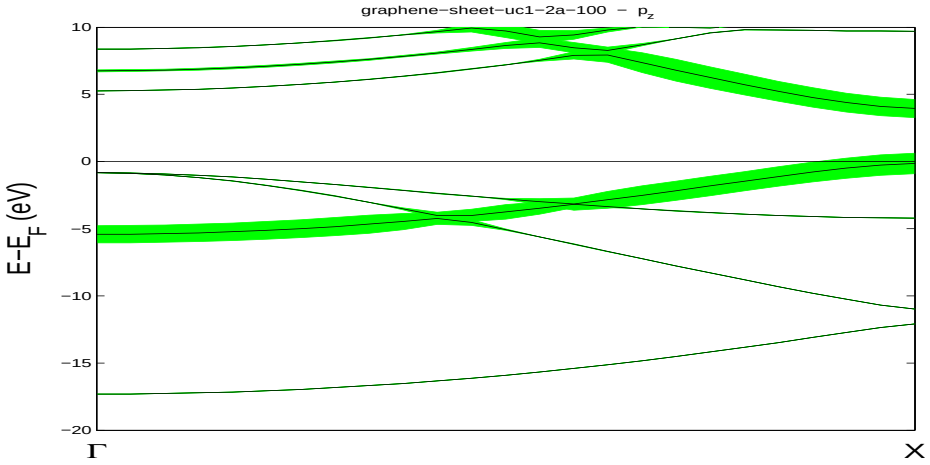
- Band structure of graphene
- Electronic structure: sp^2= π states and σ states.
- π states at E_{Fermi}

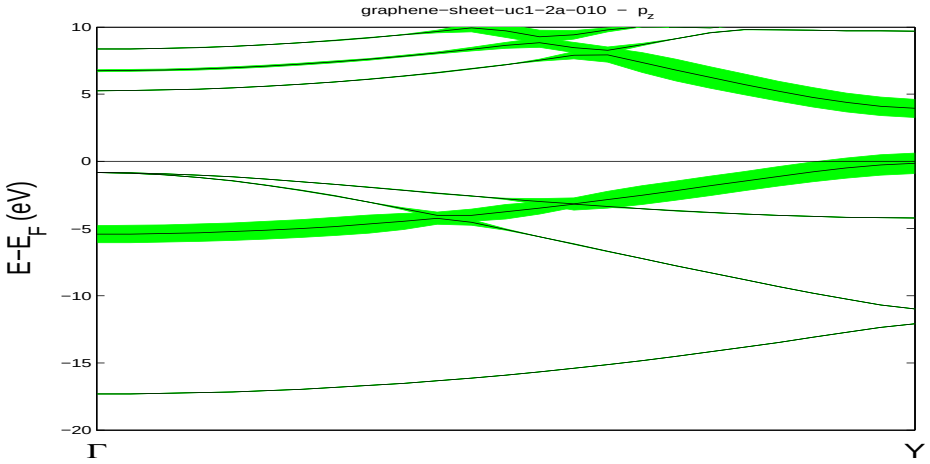
Graphene II



- Density of States of graphene.
- π states at E_{Fermi}

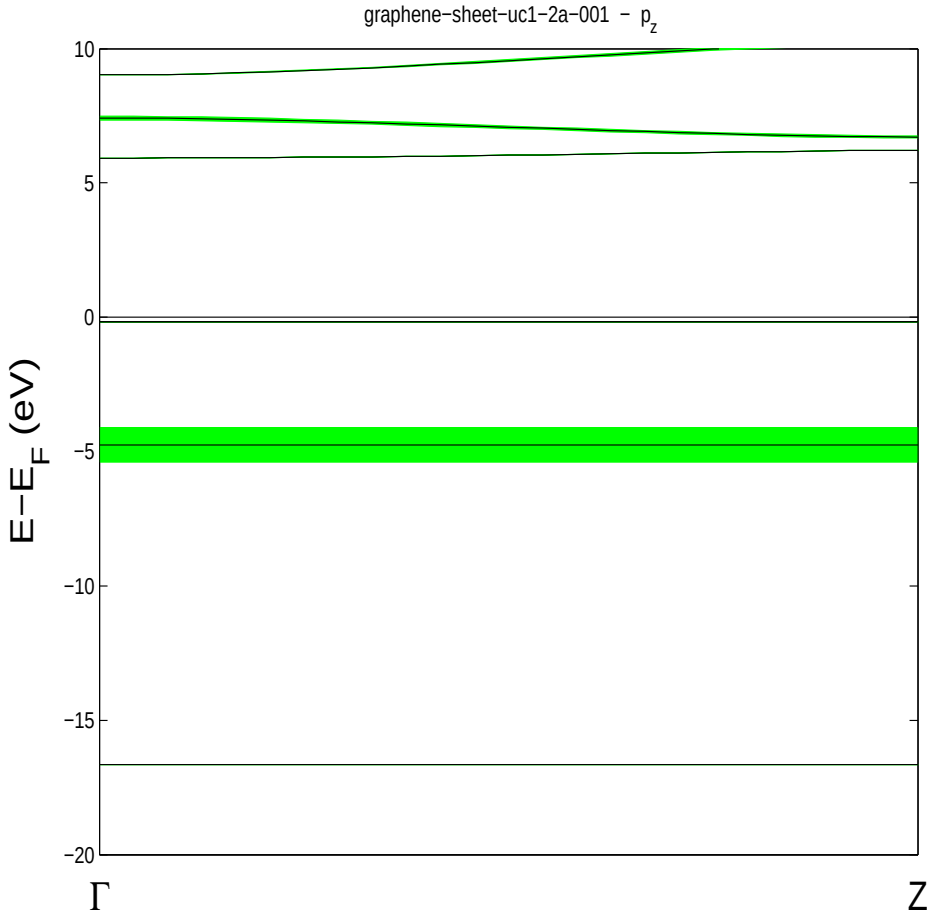
Graphene III





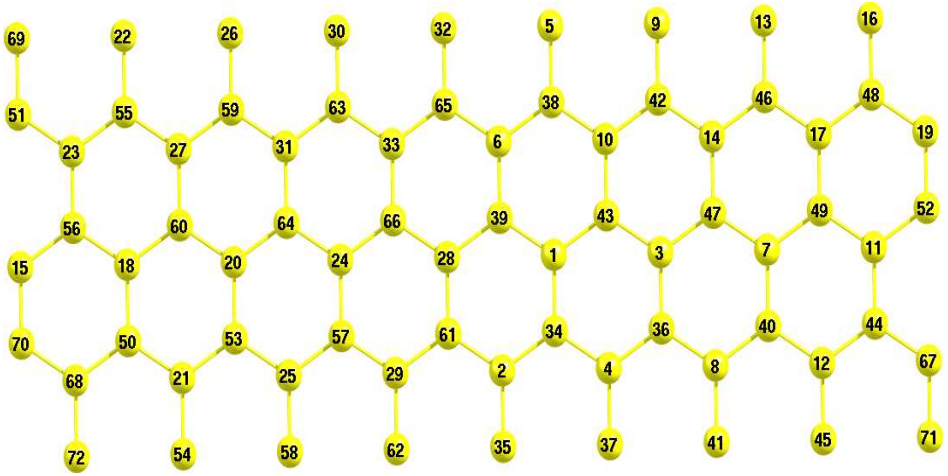
- Band structures of graphene in X- and Y-directions along the unit cell.
- They are the same and semiconducting in these directions.
- π states shown in green.

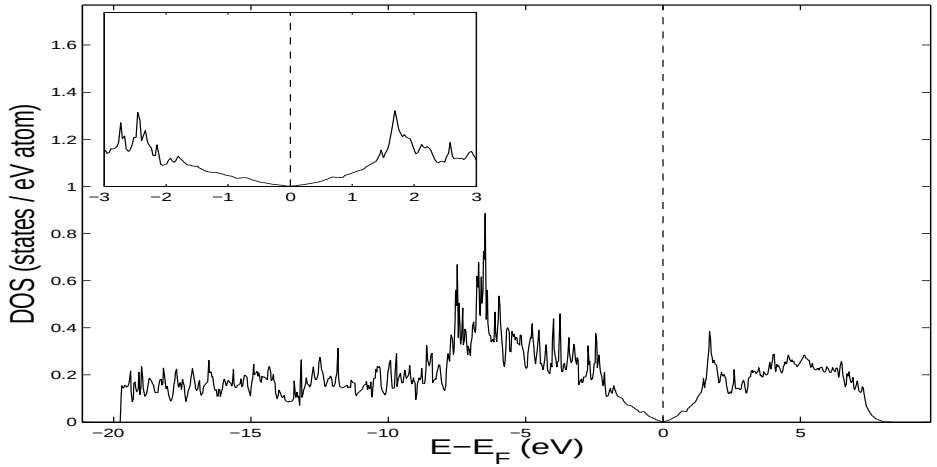
Graphene IV



- Band structures of graphene in Z-direction.
- The bands for Bloch states with $\overrightarrow{k}$-vectors are flat.
- Due to a large lattice parameter chosen to isolate them from neighboring sheets.

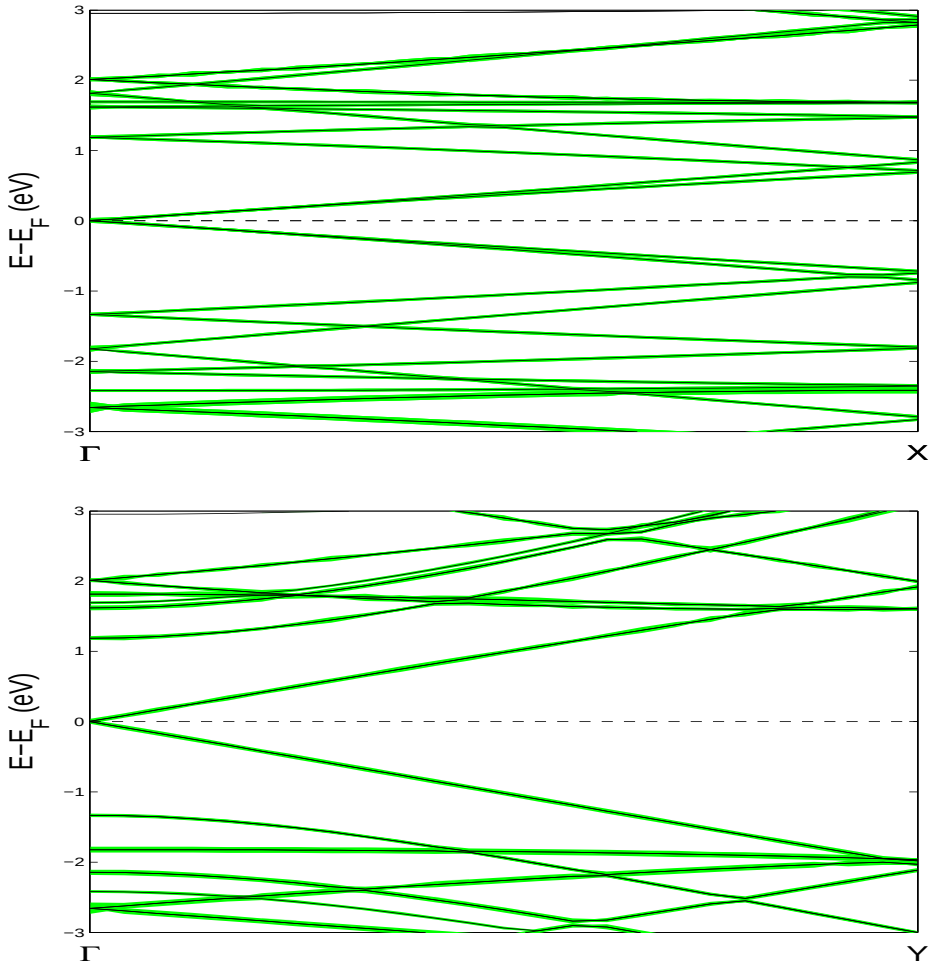
Graphene V





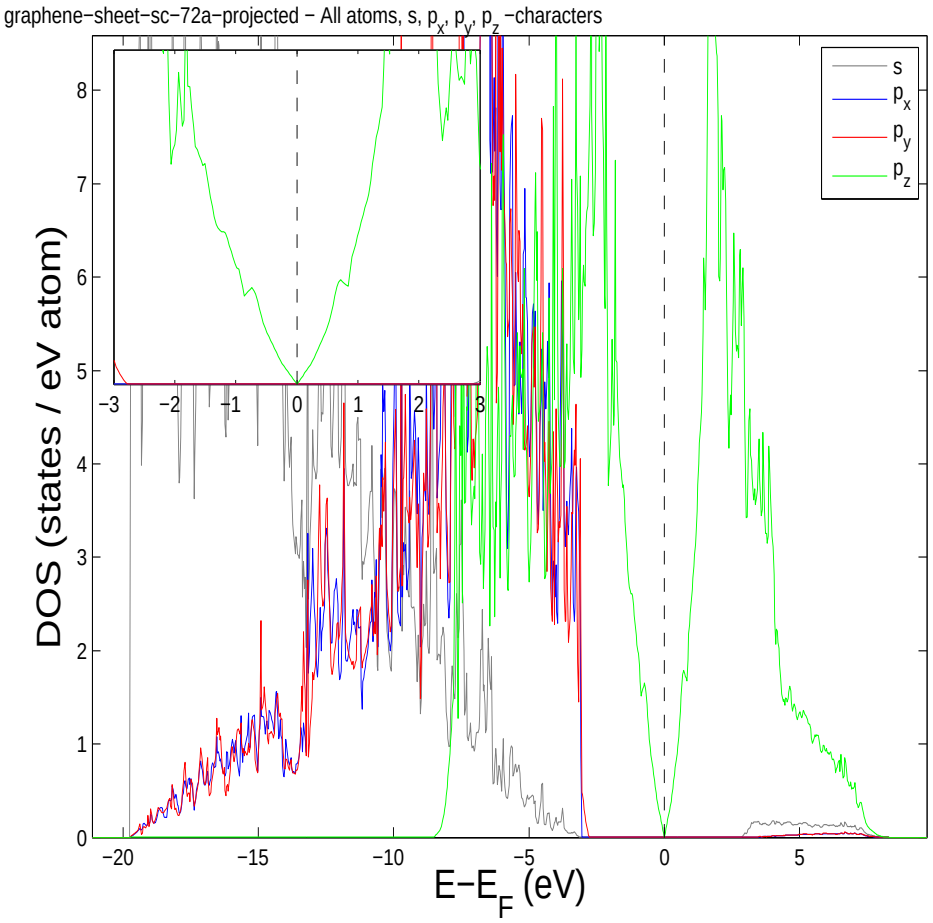
- Super cell of graphene with 72 atoms.
- Density of States of graphene.
- No (very small!) band gap at E_{Fermi}.
- Same properties with conventional two atoms unit cell.

Graphene VI



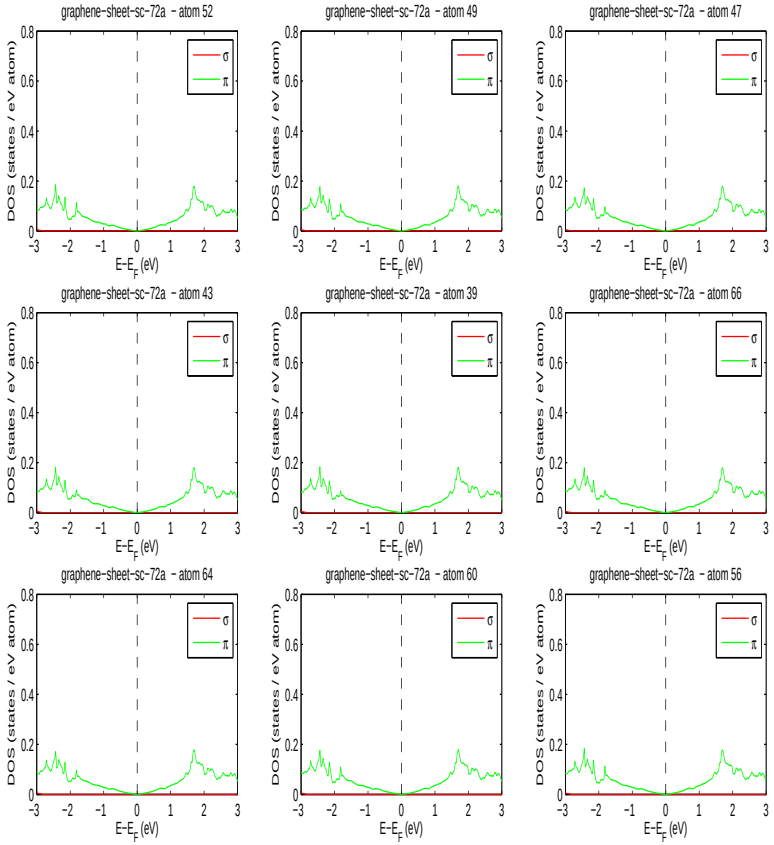
- Band structures of graphene in X- and Y-directions along the super cell.
- They are not the same due to asymmetry in super cell.
- π states shown in green.
- Band gap increases when deviate from Γ-point.

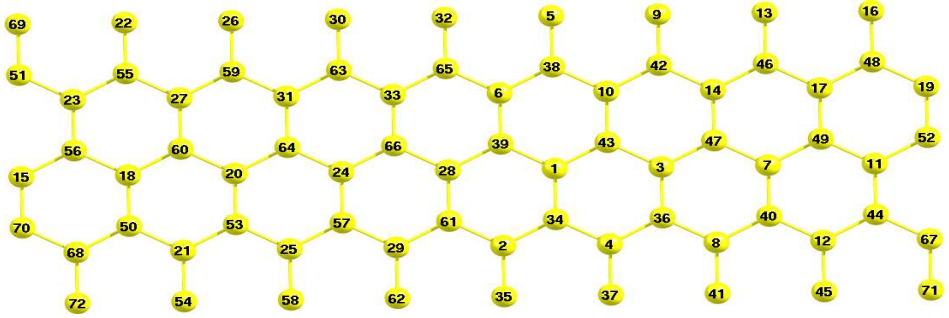
Graphene VII



- Density of States (DOS) of graphene with projection of electronic states.
- π states at E_{Fermi}

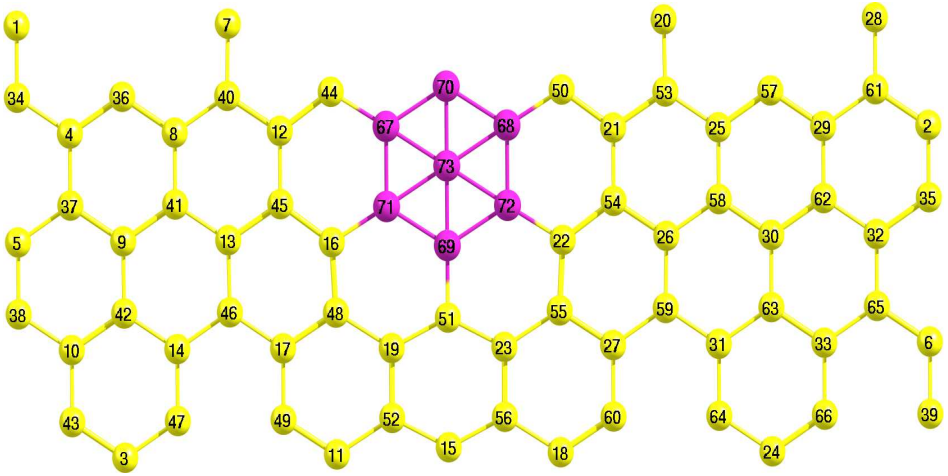
Graphene VIII

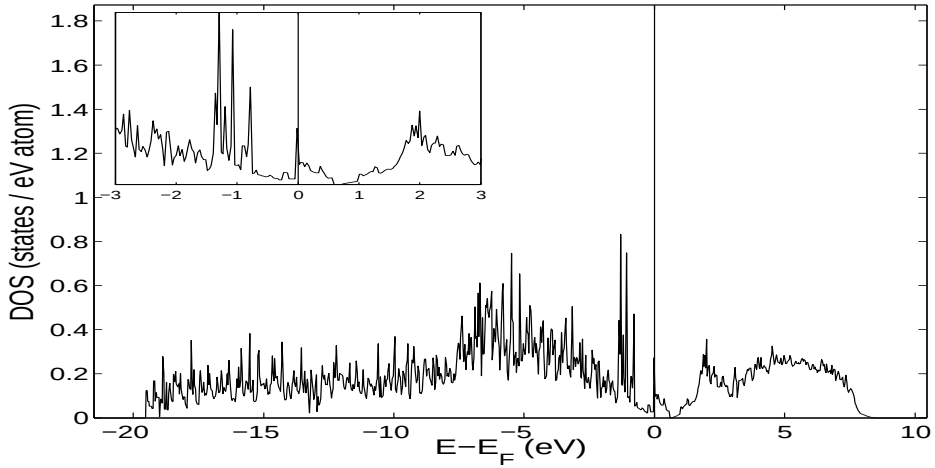




- Projected DOSs for graphene.
- $\sigma = s + p_x + p_y$ & $\pi = p_z$
- They are all same.
- And exhibit general DOS behavior.
- π states at E_{Fermi}

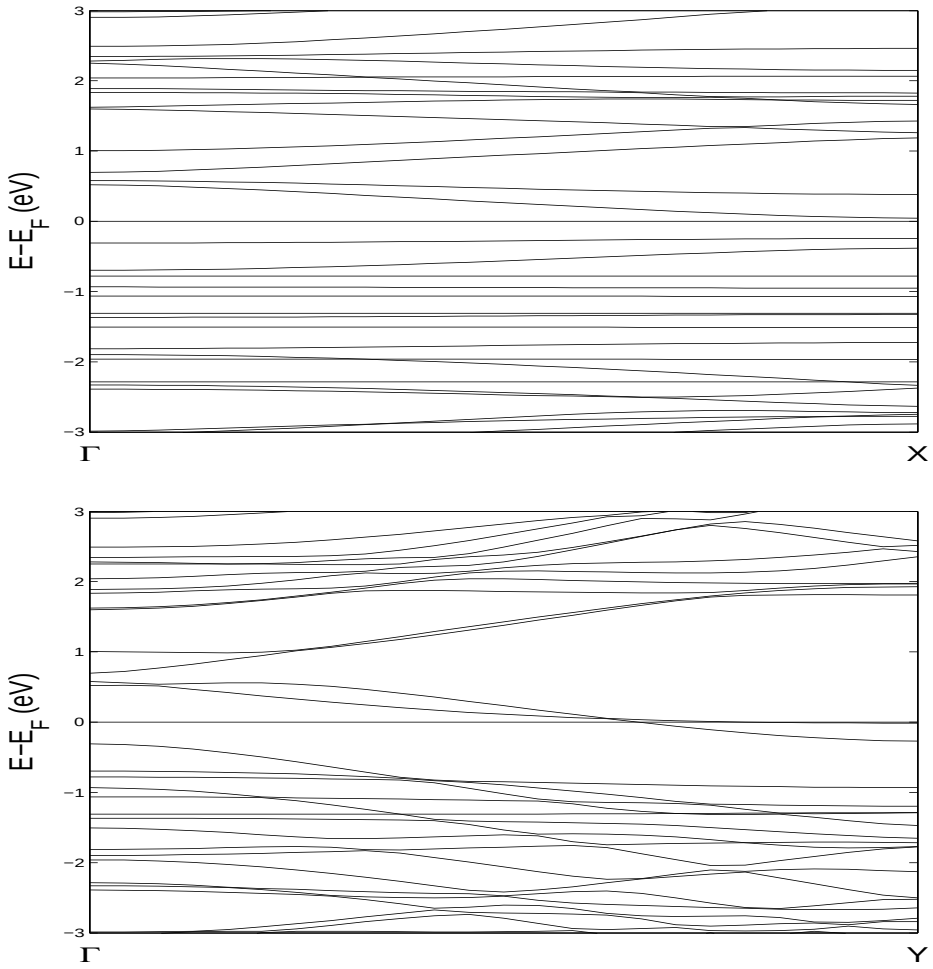
Boron Doped Graphene I





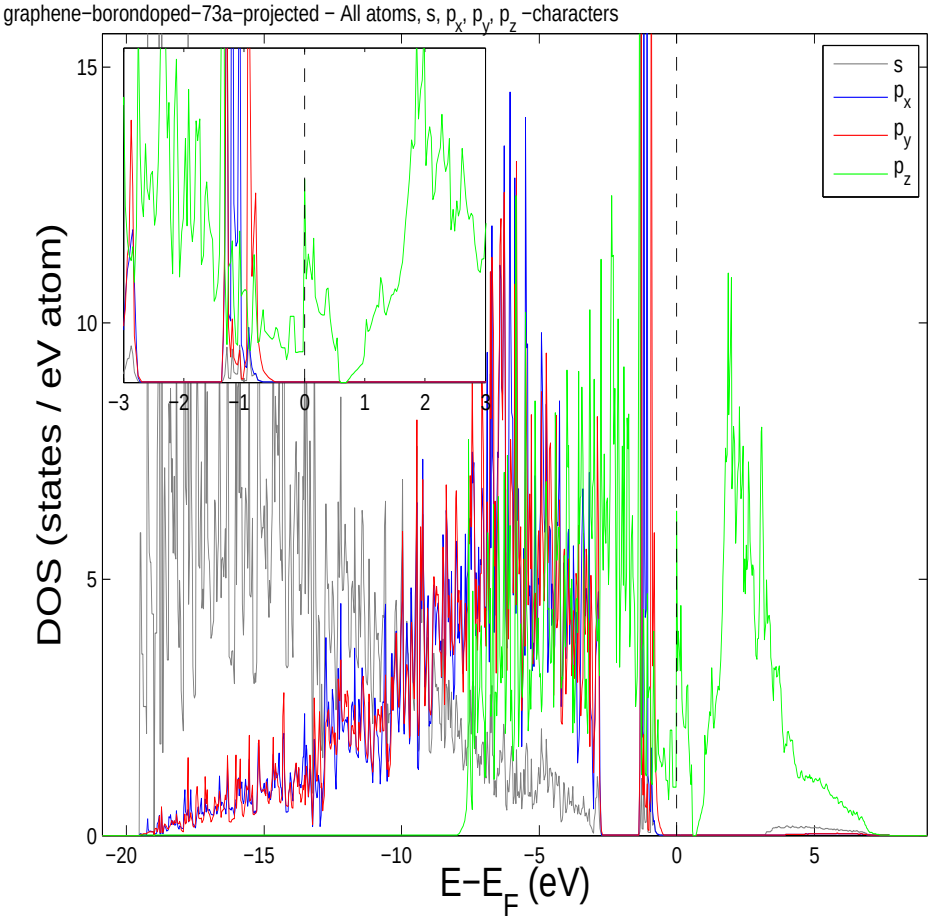
- B_7-cluster is accepted by graphene matrix.
- Linear chains of alternating $B_7 - C_6$ clusters.
- Electronic structure about $E_F = 0$ is altered.
- Boron metallizes the graphene.

Boron Doped Graphene II



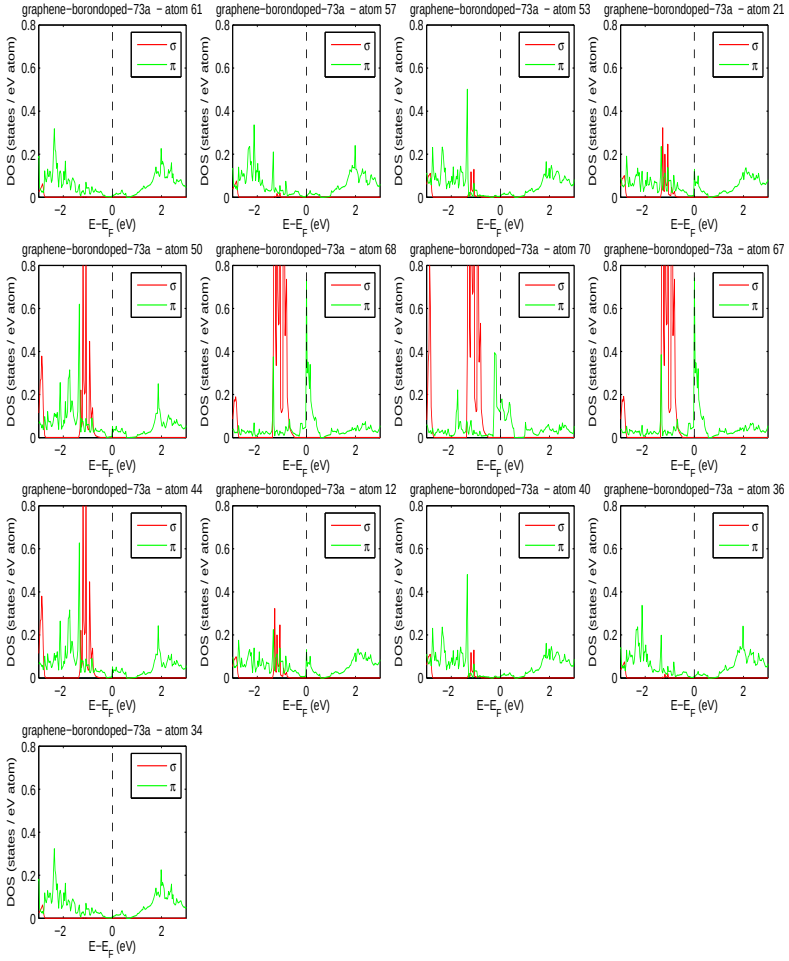
- Band structures of boron doped graphene along the super cell.
- Conduction band pulled down towards the Fermi level for Bloch states with $\overrightarrow{k}$-vectors in x-direction.
- Might be coupled to Bloch states with $\overrightarrow{k}$-vectors in the vertical y-direction.
- Metallic behavior of the underlying graphene matrix.

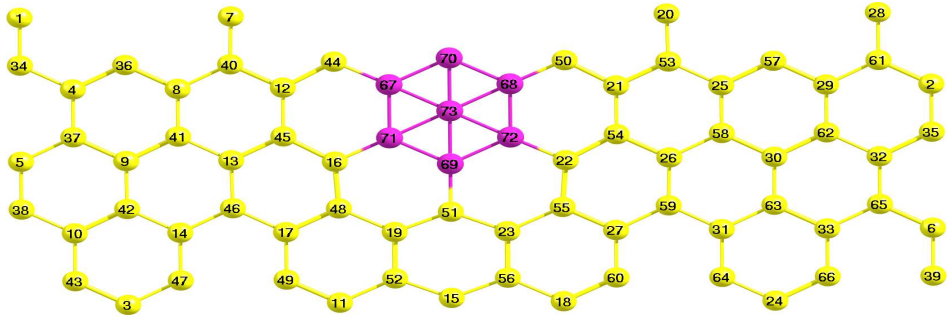
Boron Doped Graphene III



- Density of States (DOS) of graphene with projection of electronic states.
- π states at E_{Fermi}

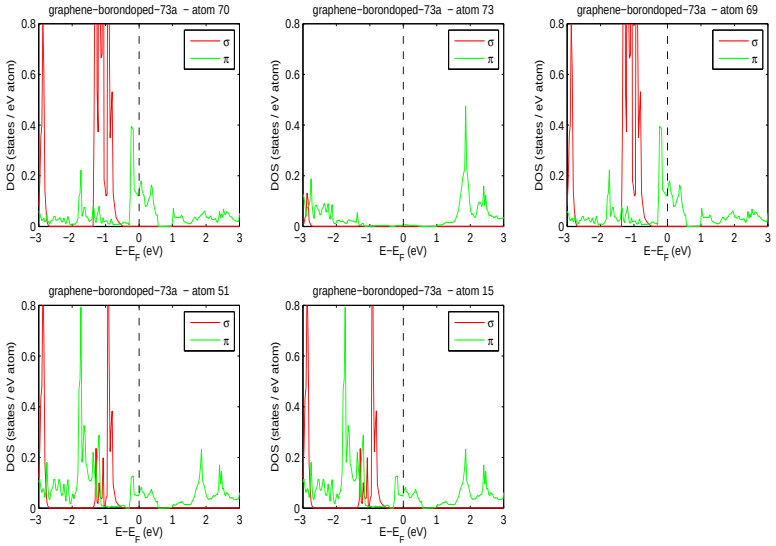
Boron Doped Graphene IV

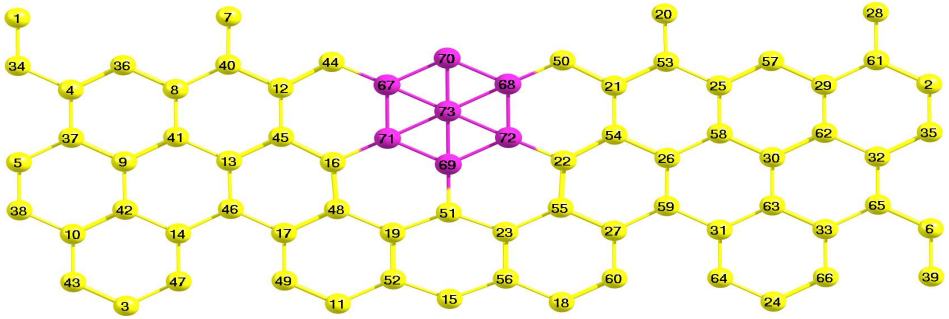




- Projected DOSs for boron doped graphene.
- Transverse direction.
- Metallicity on the outer B atoms and within a shell of first and second nearest neighbor C atoms.

Boron Doped Graphene V





- Periodic direction.
- Central B atom does not contribute.
- $B_7 - C_6$ chain along the periodic direction forms a metallic wire.

Summary

- A proposed model system for a route to nanoelectronics.
- Semiconducting graphene substrate + chains of boron clusters for wiring.
- Theoretically studied within the framework of DFT.
- Graphene matrix easily accepts these alternating $B_7 - C_6$ chains.
- Semiconducting properties might be supplemented by parts of the graphene matrix itself.
- Chains of boron clusters form a metallic wire inside the semiconducting graphene matrix.

Future Works

- Determination of the distance between boron clusters in the periodic direction, where the metallic behavior might finally disappear.
- Implantation of even larger boron clusters.
- Modeling of inhomogeneous or disordered cluster chains.