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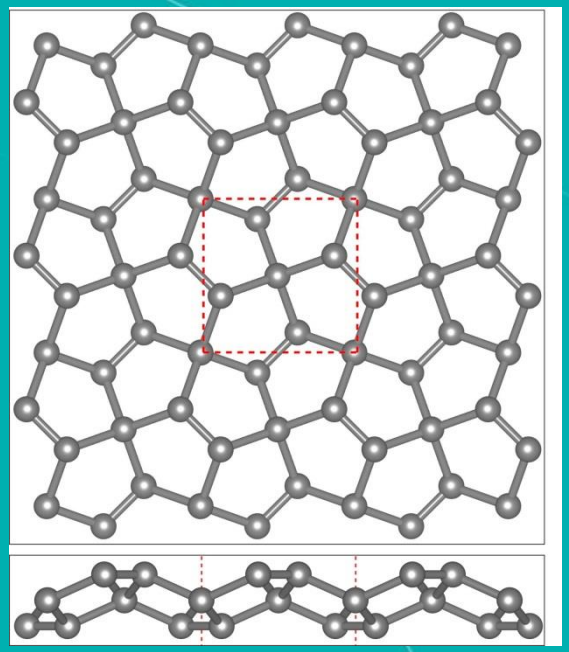
البيئة والطاقة
Qatar Environment & Energy
Research Institute

جامعة حمد بن خليفة
HAMAD BIN KHALIFA UNIVERSITY

Band gap engineering in penta-graphene by substitutional doping

Golibjon Berdiyorov



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QEERI counts with 132 full time staff (as of March 2016), from which 92 are PhD holders of 43 different nationalities. These world-class researchers focus their efforts on 29 Grand Challenge Projects and 33 sponsored projects

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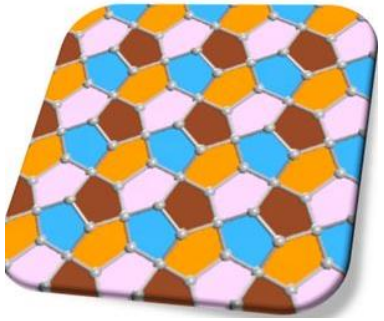
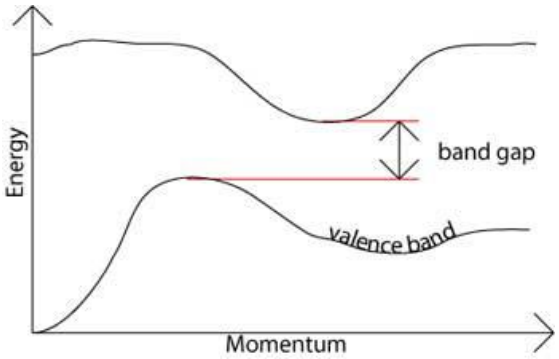
- Energy Storage
- Material Sciences and Engineering
- Water Desalination and Treatment
- Environmental and Chemical Sciences
- Theory, Modeling and Simulation
- Imaging, Characterization and Analytics
- Measurements Science and Analytics
- Special Projects

Outline

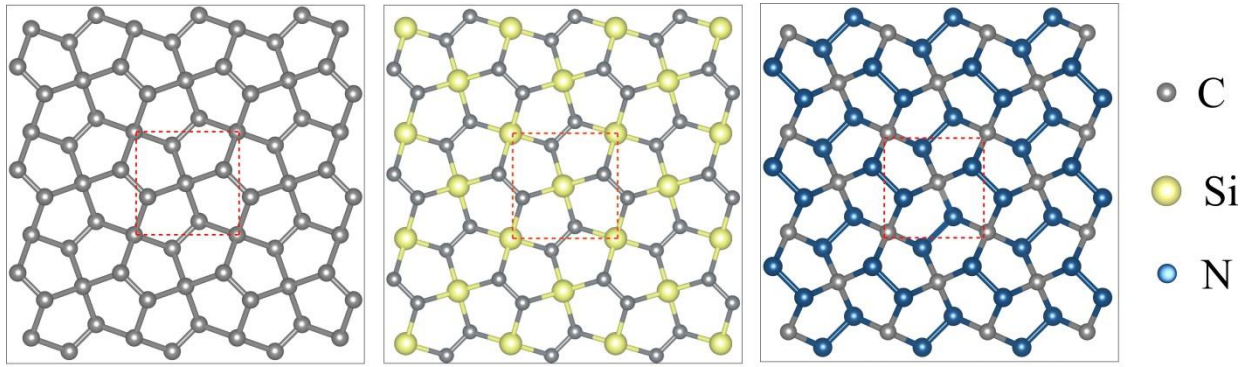


- Introduction
  - Penta-graphene: a new carbon allotrope
  - Motivation and objectives

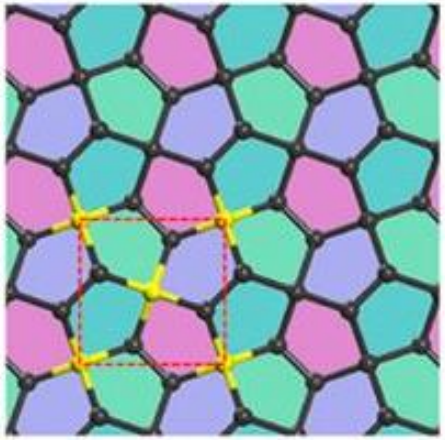
- Theoretical approach $H\psi$
- Results
  - Band-gap engineering in penta-graphene: substitutional doping vs. surface termination
  - Optical and transport properties of penta-graphene, penta-SiC_2 and penta-CN_2



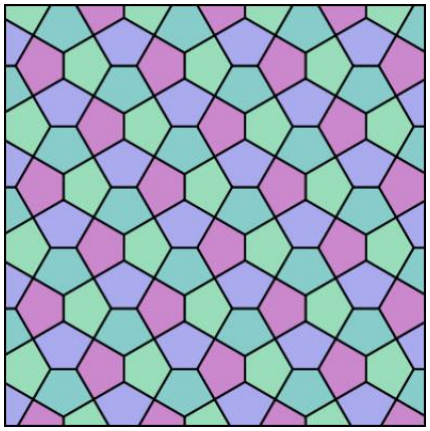
- Conclusions



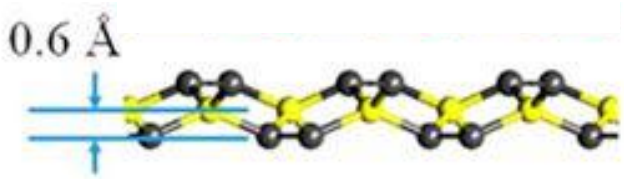
Introduction: Penta-graphene



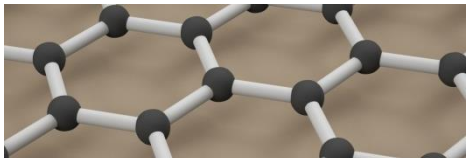
Penta-graphene: 2D carbon allotrope composed exclusively of pentagons.

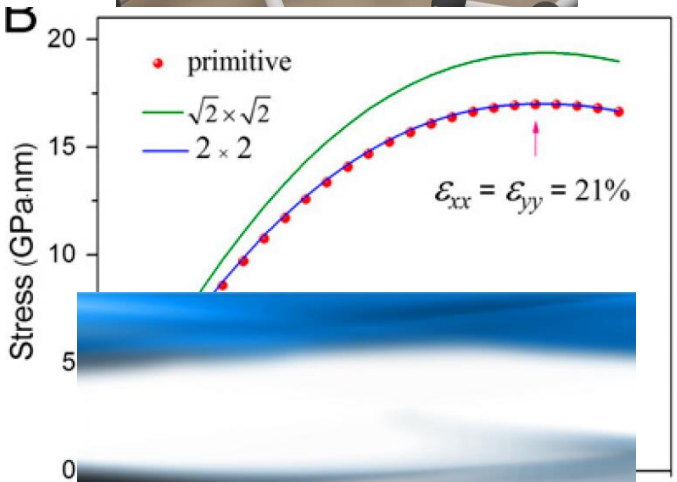


Cairo tile pattern: pentagons are not regular, otherwise can not tile a surface



a mixture of sp^2- and sp^3-coordinated carbon atoms

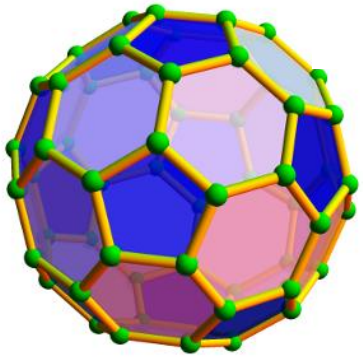


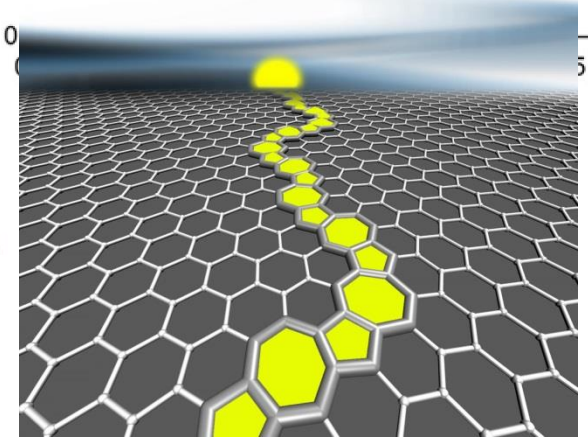


Zhang et al. Proc.Natl. Acad. Sci. U. S. A. ***112,*** *2372 (2015).*

- Dynamically and mechanically stable and withstands temperatures up to 1000 K.
- Unusual negative Poisson ' s ratio
- Ultrahigh strength that can even outperf
- **Wide-gap semiconductor (3.25 eV).**

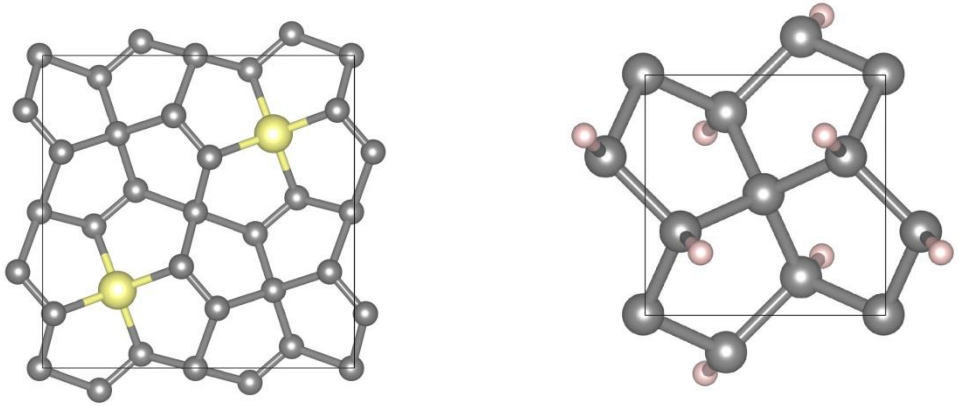
Experimental realization!?



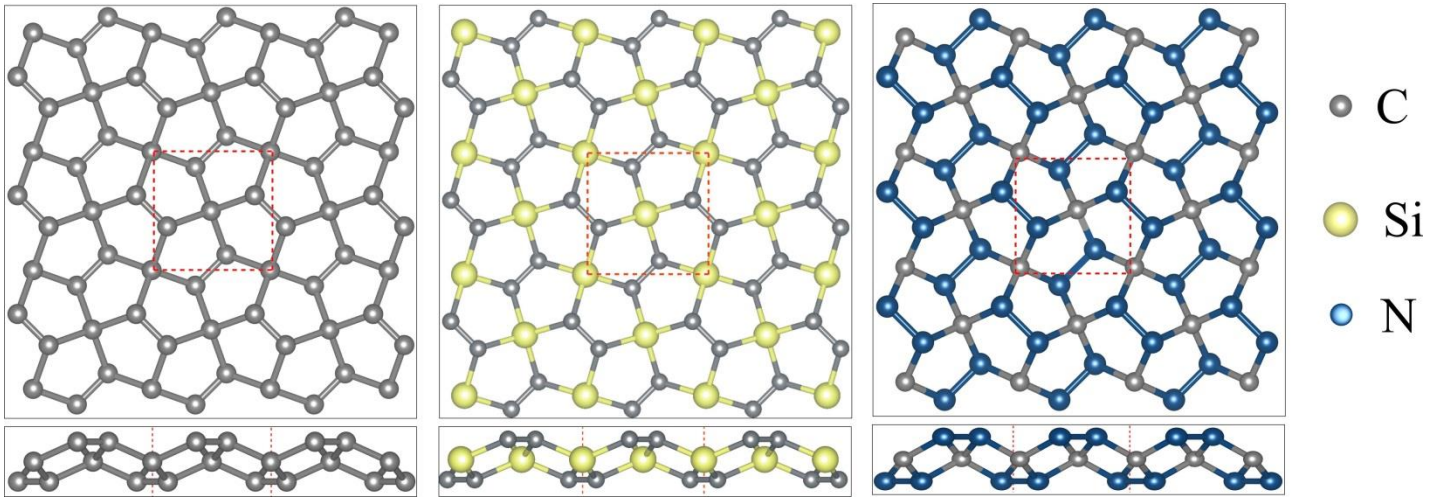


Objectives

- Band gap engineering



- Electronic transport and optical properties



Penta-SiC_2 Penta-CN_2

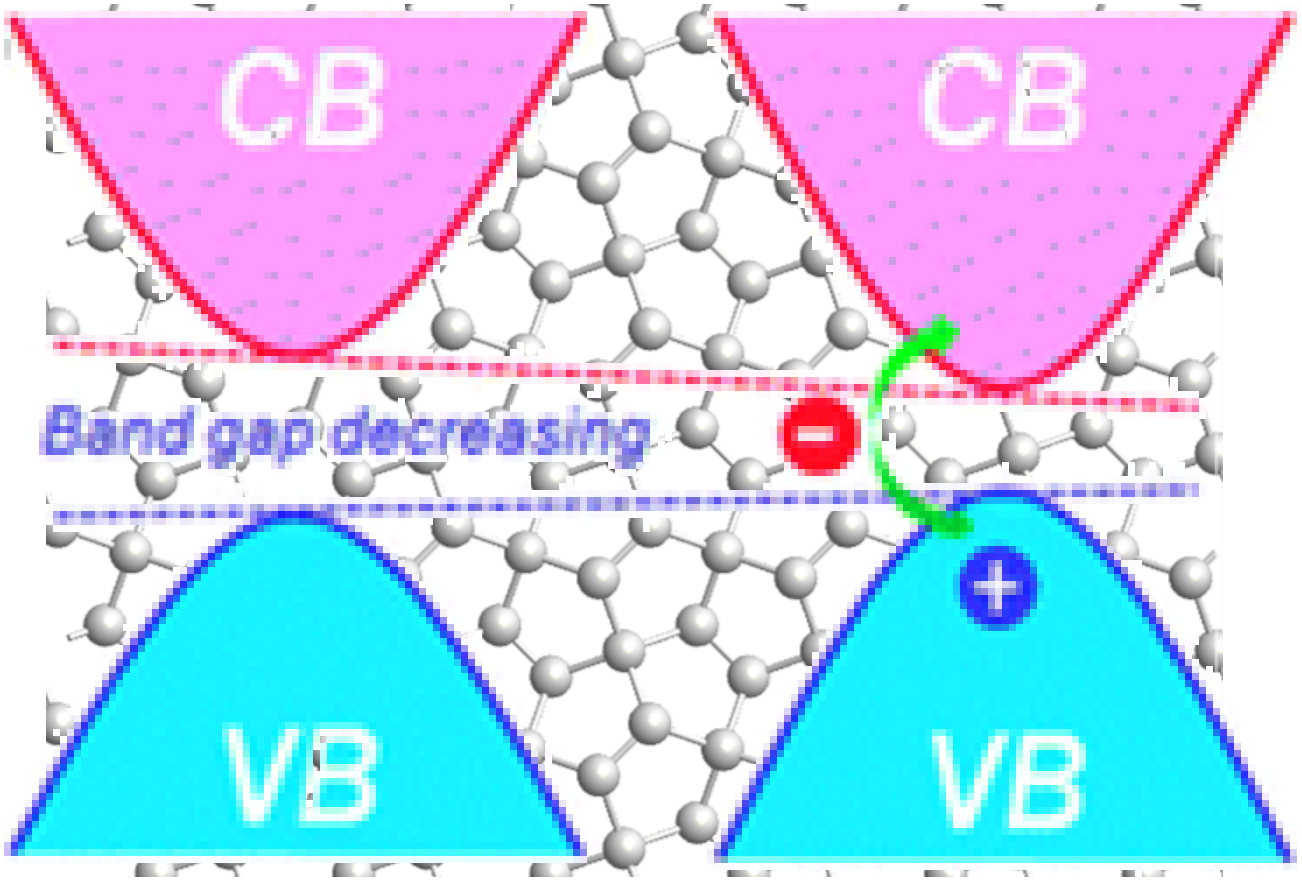
Lopez-Bezanilla and Littlewood, J. Phys. Chem. C **119**, 19469 (2015).
Zhang et al., J. Phys. Chem. C **120** , 3993 (2016).

Approaches used

- DFT (GGA:PBE): structural analysis and electronic properties (van der Waals interactions).

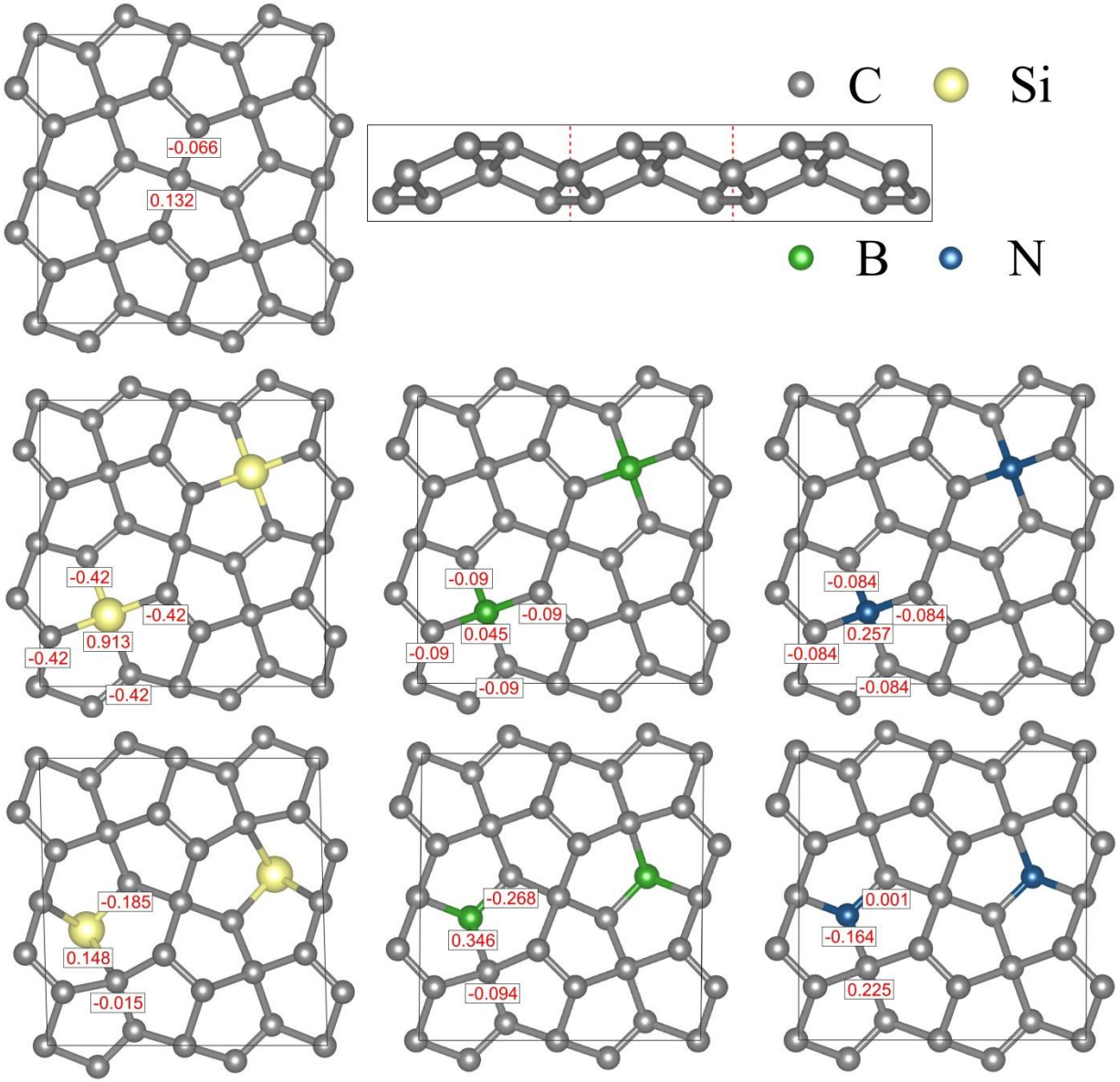
- Quantum transport: nonequilibrium Green's function formalism.

Part I
Band Gap Engineering



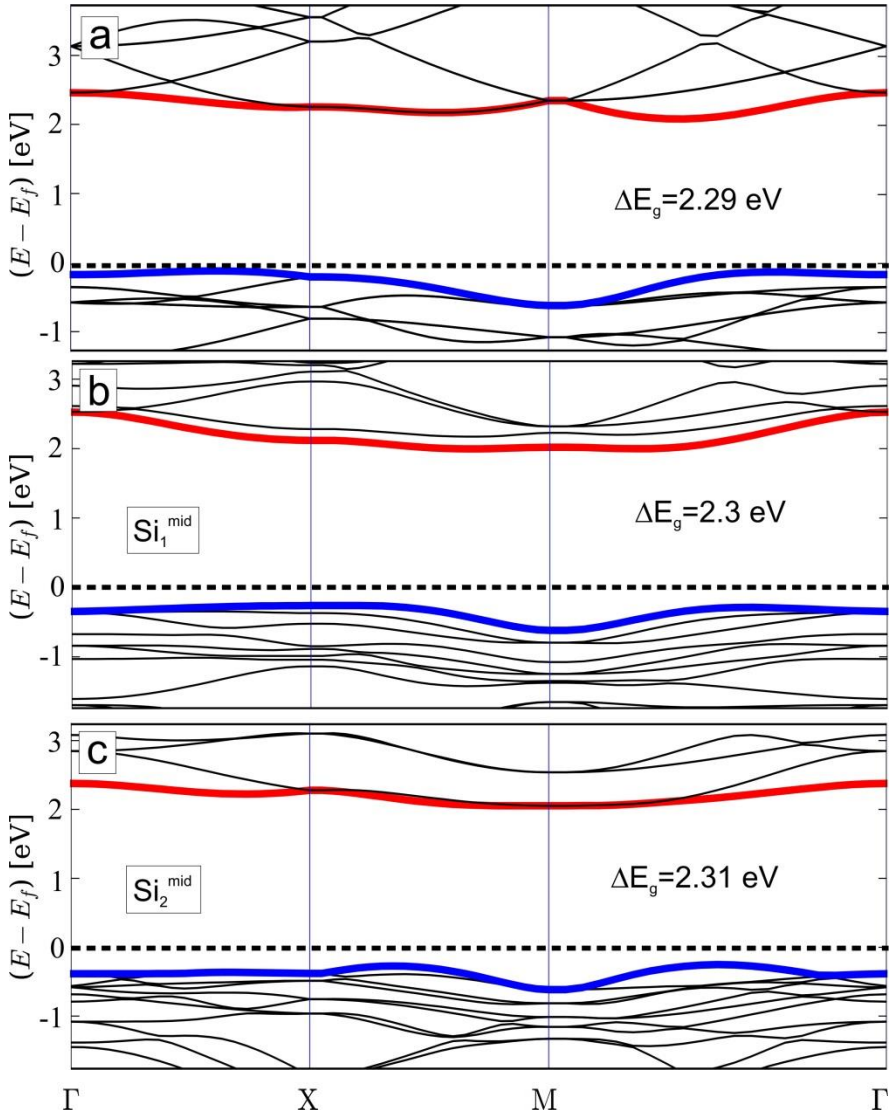
Berdiyorov et al., Journal of Physics: Condensed Matter (2016)

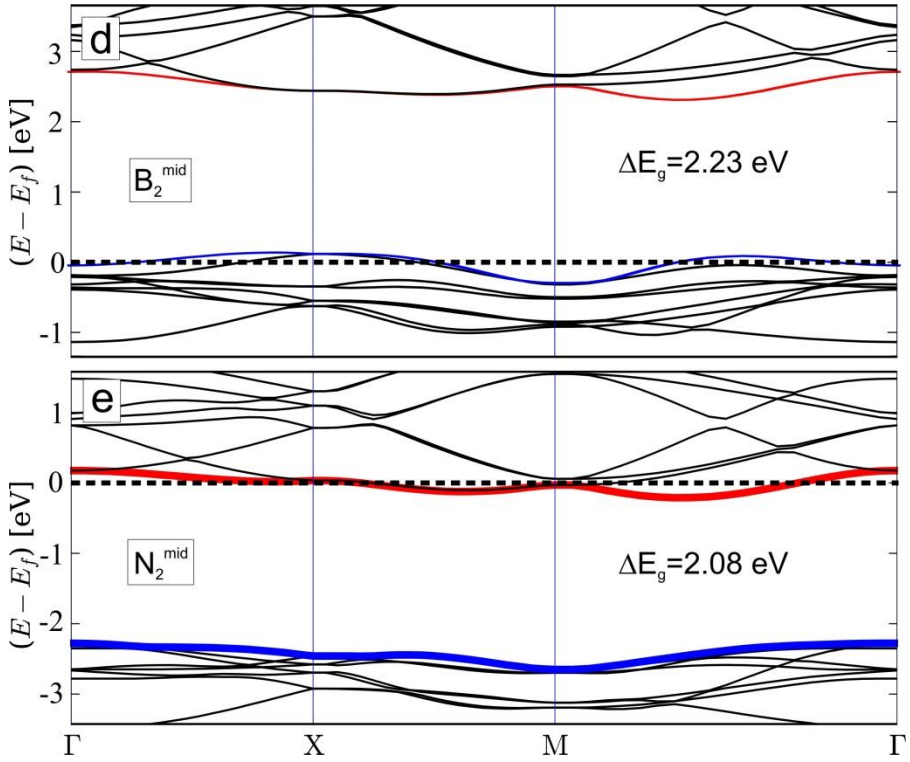
Substitutional doping



Atomistic structure of pristine and doped penta-graphene. Numbers show the DDEC partial charges of the corresponding atoms.

Band structure: middle plane doping

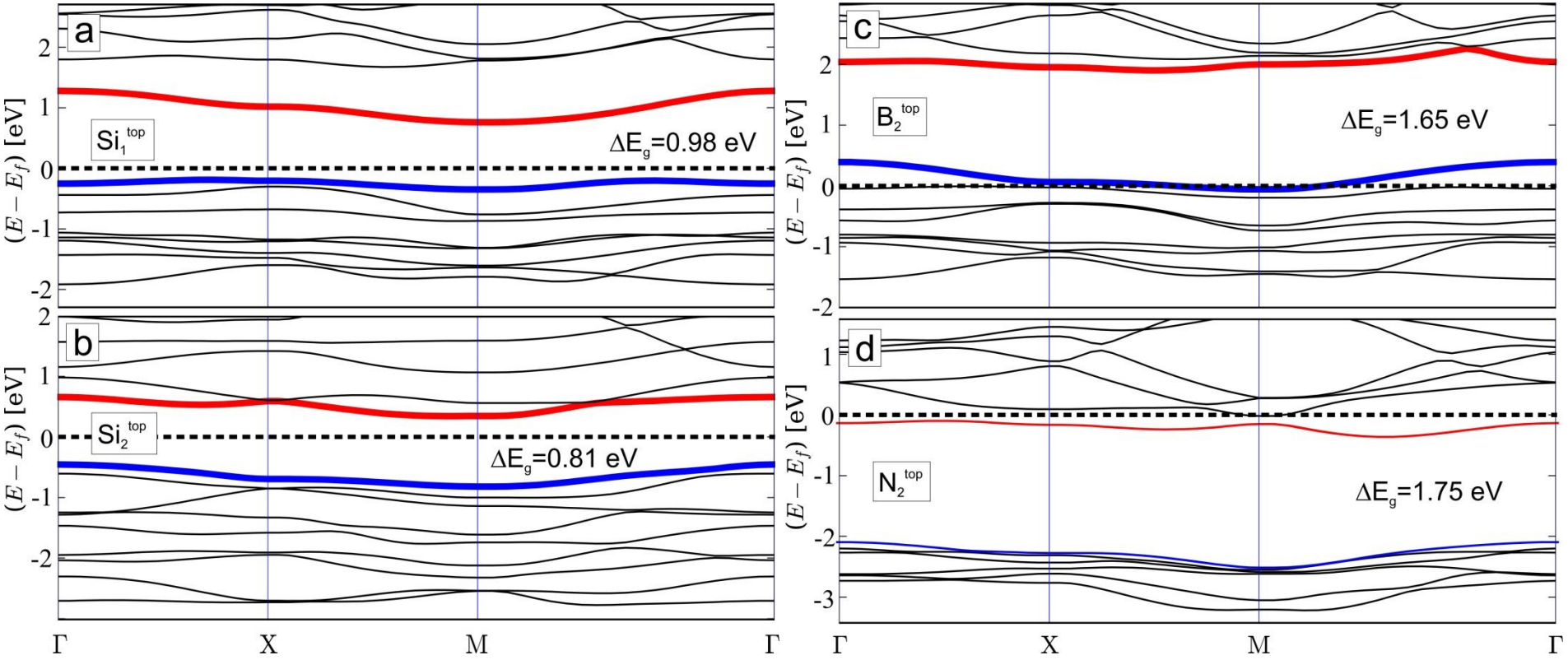




- The gap is not affected much by middle plane doping.

Band structure of penta-graphene without (a) and with substitutional doping (b-e) in the middle plane: single Si (b), double Si (c), double B (d) and double N (e). The Fermi energy and band gap values are gives in each panel.

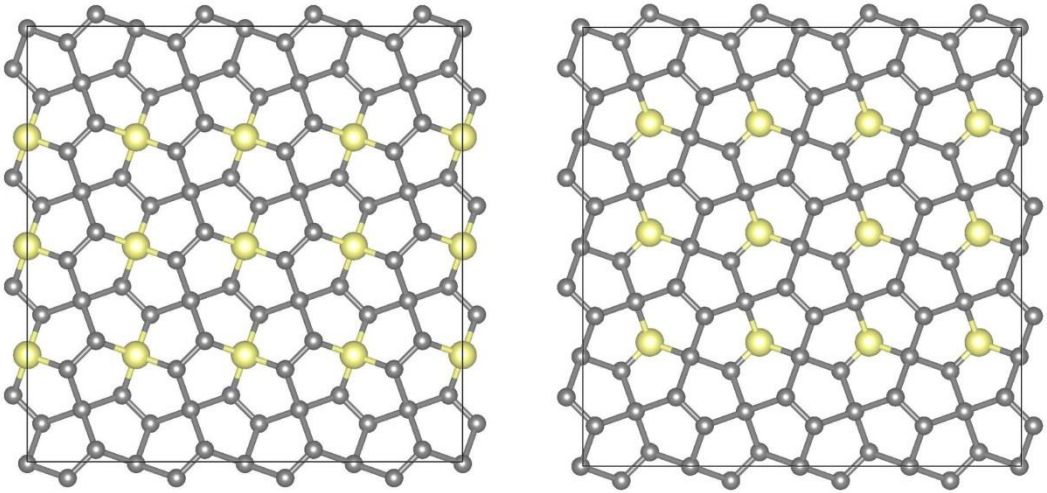
Band structure: top/bottom plane doping

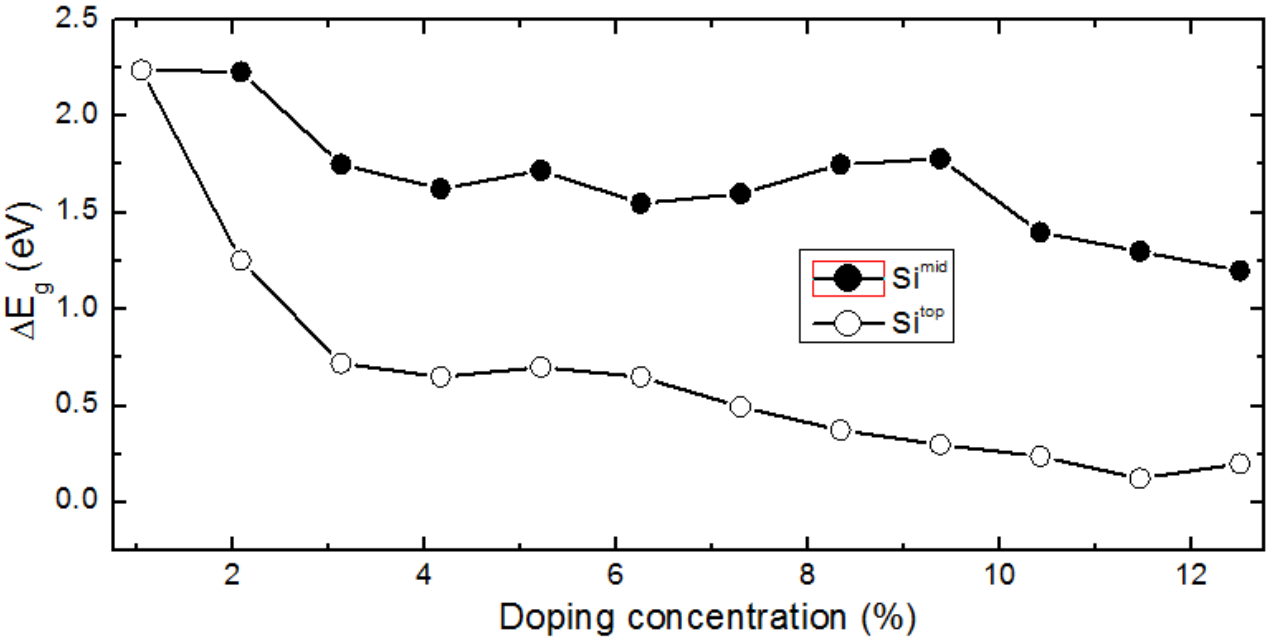


- The electronic band gap is strongly reduced due to the doping.
- Si atoms are more effective.

Band structure of penta-graphene with substitutional doping on the top (bottom) plane: single Si (a), double Si (b), double B (c) and double N (d).

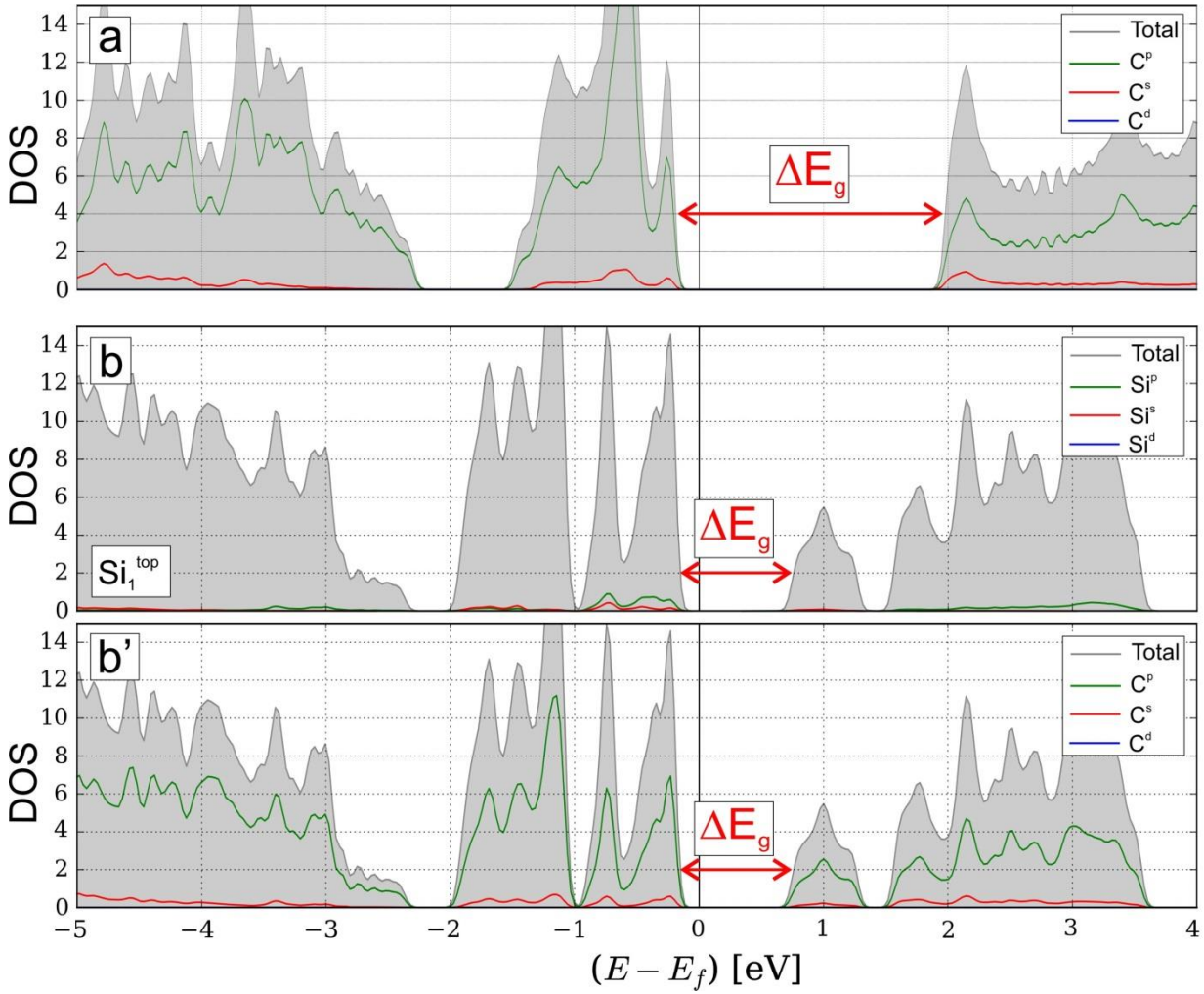
Effect of doping concentration





Optimized structure of penta-graphene with 12.5% Si doping and the electronic band gap ΔE g of Si doped penta-graphene as a function of doping concentration.

DOS calculations



Density of states (DOS) of pristine penta-graphene (a) and penta-graphene with a single Si-doping on the top (bottom) plane.

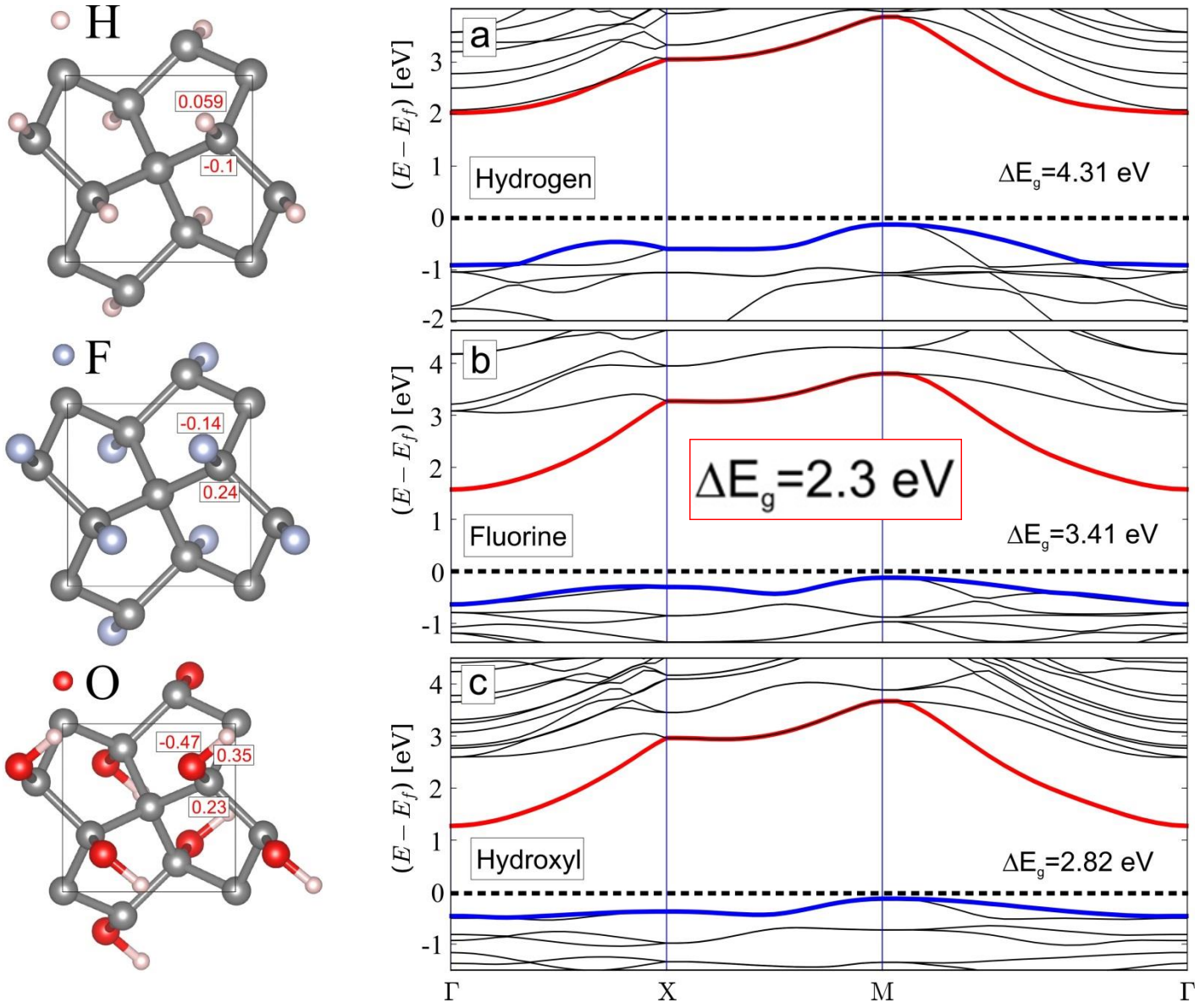
HSE calculations

TABLE I: The electronic band gap ΔE_g (eV) of substitutionally doped penta-graphene obtained using two different exchange-correlation functionals.

	PBE	HSE06
Pristine PG	2.29	3.21
Si_1^{top}	0.98	1.59
Si_2^{top}	0.81	1.01
B_2^{top}	1.65	1.79
N_2^{top}	1.75	2.33

- Results are robust against the usage of hybrid functionals.

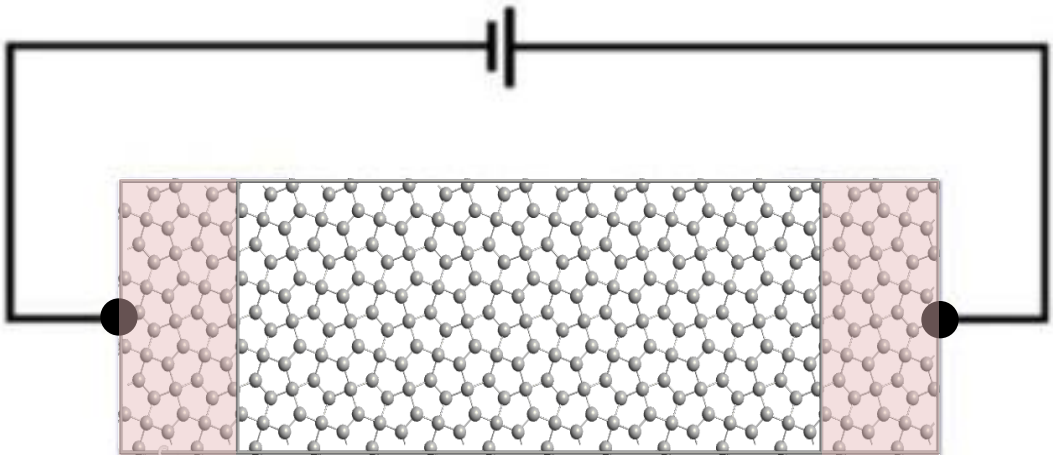
Surface functionalization



- Surface termination results in the increase in the band gap.

Part II
Electronic transport and optical properties

Ballistic transport (Landauer-Büttiker formalism)



Susceptibility tensor (Kubo-Greenwood formula)

$$\chi_{i,j}(\omega) = -\frac{e^2\hbar^4}{m^2\varepsilon_0 V\omega^2}\sum_{nm}\frac{f(E_m)-f(E_n)}{E_{nm}-\hbar\omega-i\hbar\Gamma}\pi^i_{nm}\pi^j_{mn}$$

Berdiyorov et al., RSC Adv. **6**, 50867 (2016)

Study systems

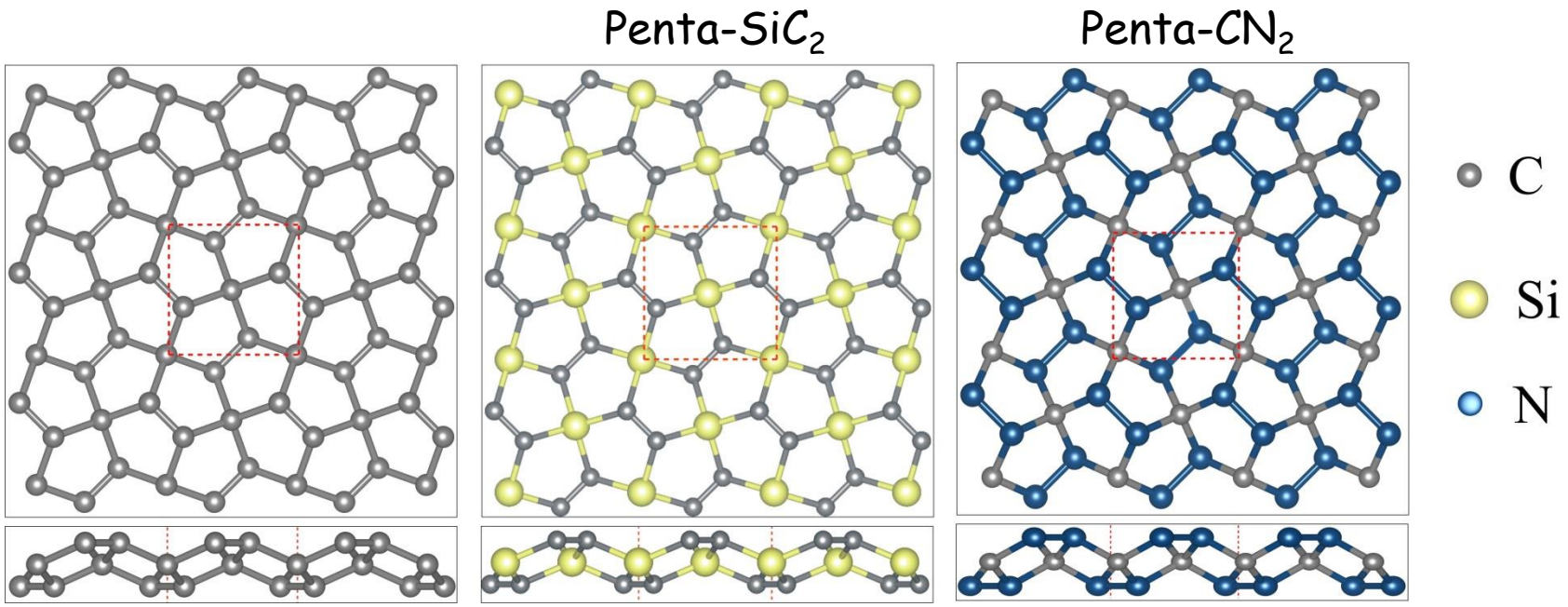
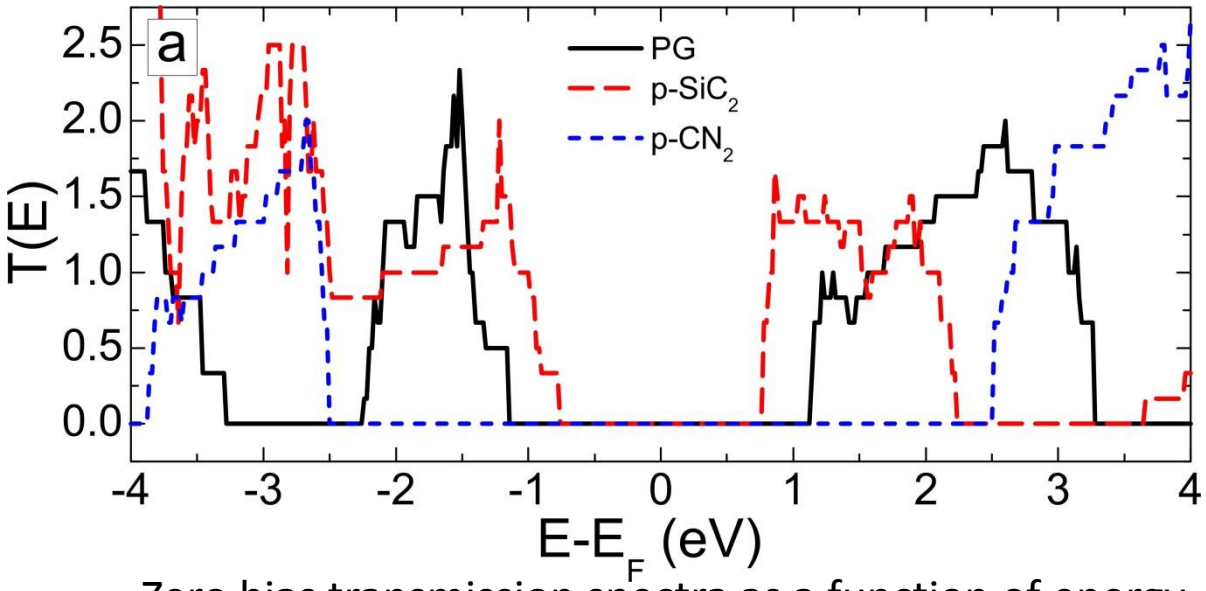


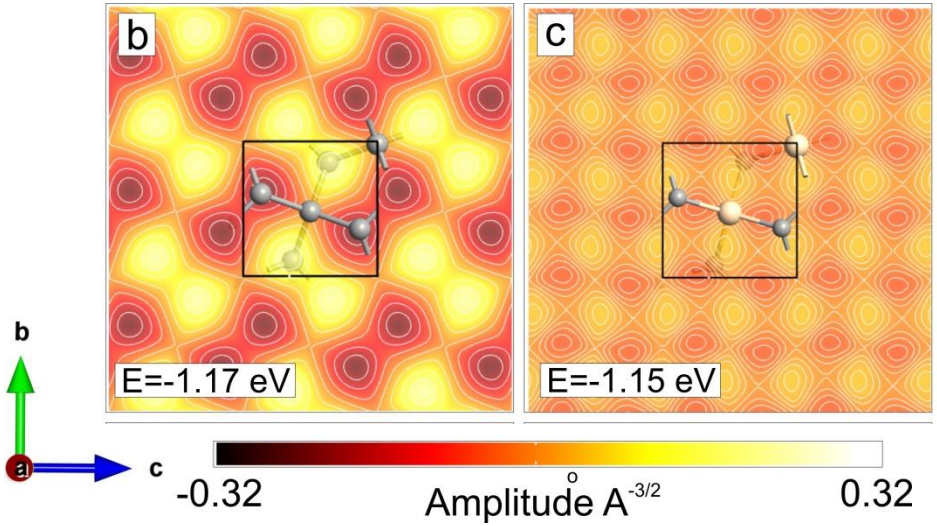
TABLE I: The lattice parameter b, thickness δ, partial charges (in the middle q(middle) and top/bottom q(top) planes) and band gaps ΔE_g (eV) (calulated using PBE and HSE06) of the considered samples.

	b (Å)	δ (Å)	q(middle)	q(top)	ΔE_g(PBE)	ΔE_g(HSE)
PG	3.639	0.608	0.132	-0.066	2.270	3.250
p-SiC_2	4.412	0.660	0.908	-0.454	1.429	2.395
p-CN_2	3.312	0.765	0.467	-0.233	4.811	6.596

Electronic transport



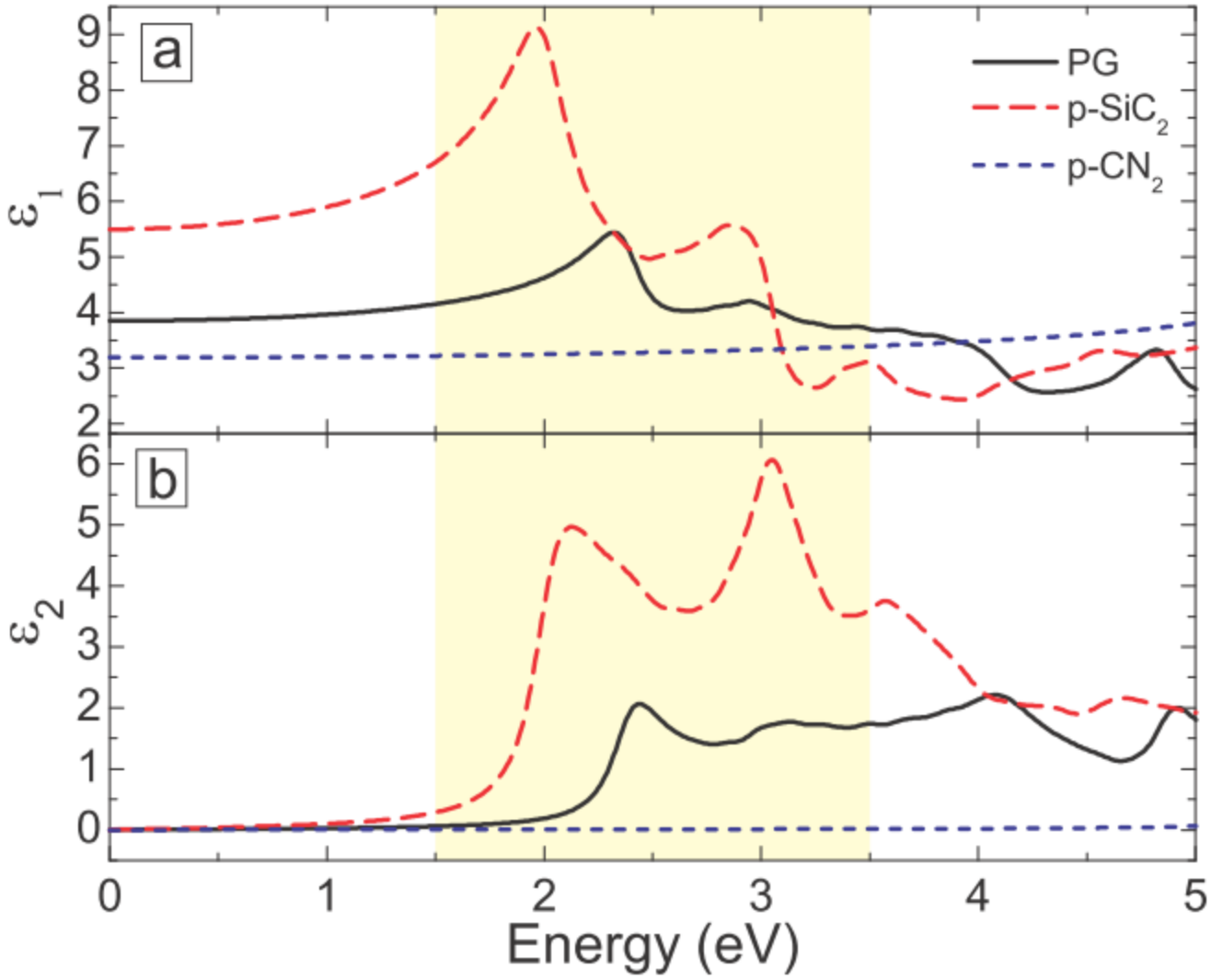
Zero bias transmission spectra as a function of energy



Contour plots of the eigenstates.

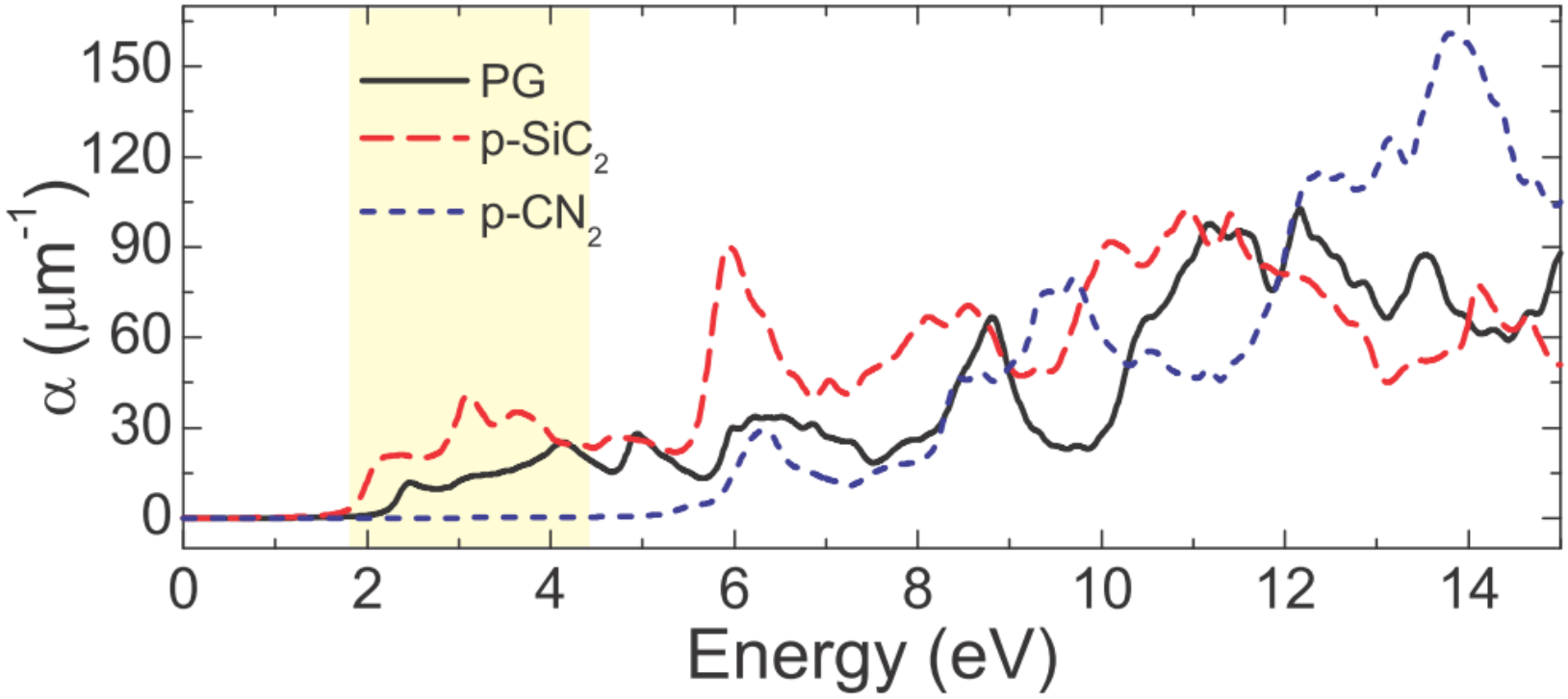
- P-SiC_2 has better electronic transport due to charge delocalization

Dielectric function



Real (ε_1) (a) and imaginary (ε_2) (b) parts of the dielectric function as functions of photon energy.

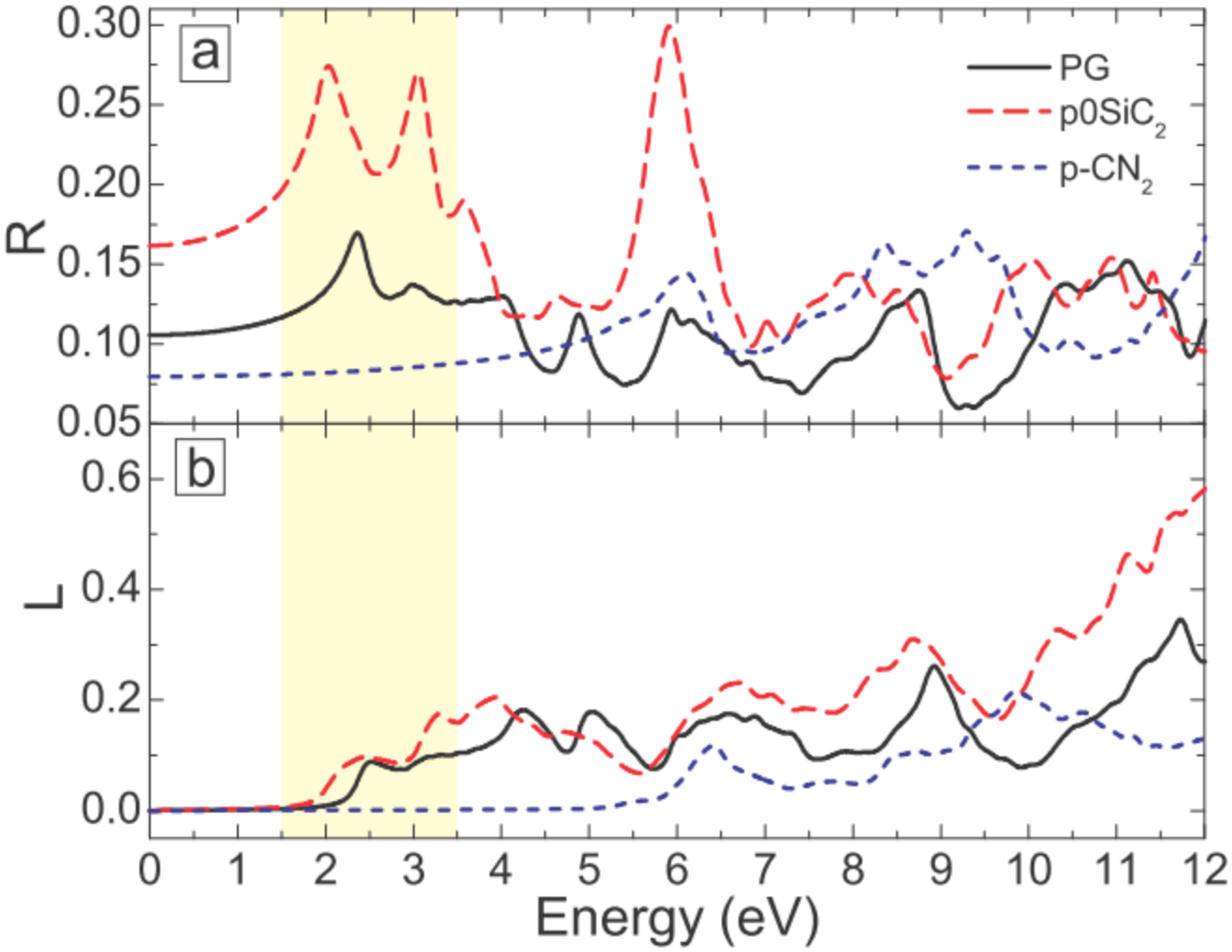
Absorption



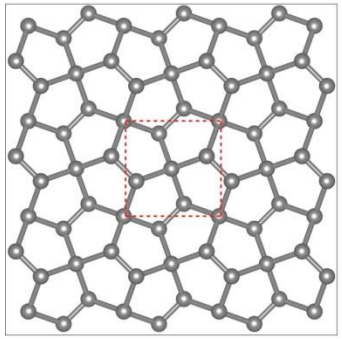
Absorption spectra as a function of photon energy

- P-SiC_2 shows better absorption in both visible and ultraviolet range of the spectrum.

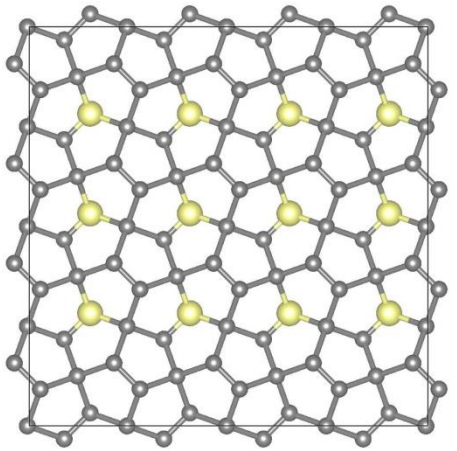
Reflectivity and loss function



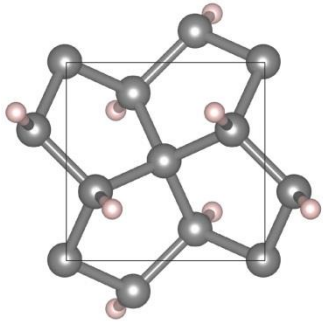
Reflectivity (a) and energy-loss spectra (b) as a function of photon energy



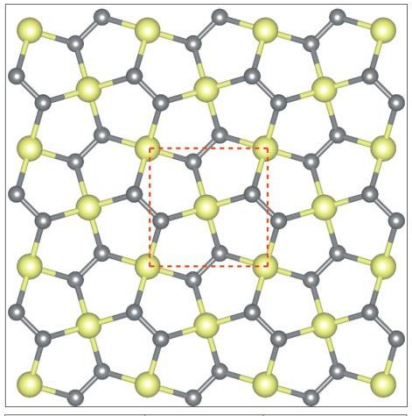
Conclusions



- Substitutional doping reduces the band gap of penta-graphene.



- Surface termination leads to an increase of the band gap.



- P-SiC_2 shows better transport and optical properties.

Acknowledgments

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King Abdullah University of Science and Technology

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Thank you!
Questions?