Density functional study of carbon mono- and bilayers on SiC

by Constanze Jahn

Overview

- Motivation
- Density functional theory
- on SiC
  - properties
  - surface reconstructions
  - Production of SiC/Graphene
  - model interface
- Graphene
- Results of the calculations:
  - SiC (0001)/ Graphene
  - SiC (000^{-}1)/ Graphene
- Outlook

Motivation

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„free standing graphene“
for electronic applications

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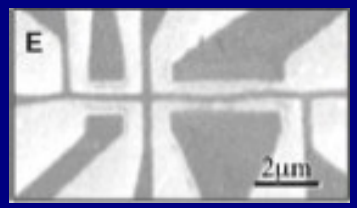
2D nano-electronics:



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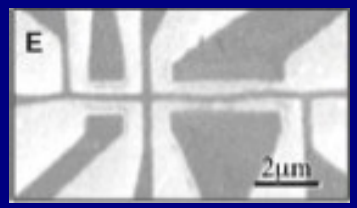

→

Interface SiC/Graphene:
- atomic structure
- electronic structure

Density functional theory

after Hohenberg, Kohn and Sham

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wavefunction $\Psi\{ (\mathbf{r}_i) \}$  density $n (\mathbf{r})$

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Kohn-Sham-formalism:

effective one particle system $\Phi_i(\mathbf{r}) \rightarrow n_0(\mathbf{r}) = \Sigma_i |\Phi_i(\mathbf{r})|^2$

$[-1/2\ \Delta + V_H[n_0](\mathbf{r}) + V_{XC}[n_0](\mathbf{r}) + V_{el}(\mathbf{r}, \{\mathbf{R}_i\})]\ \Phi_i(\mathbf{r}) = \varepsilon_i \Phi i(\mathbf{r})$

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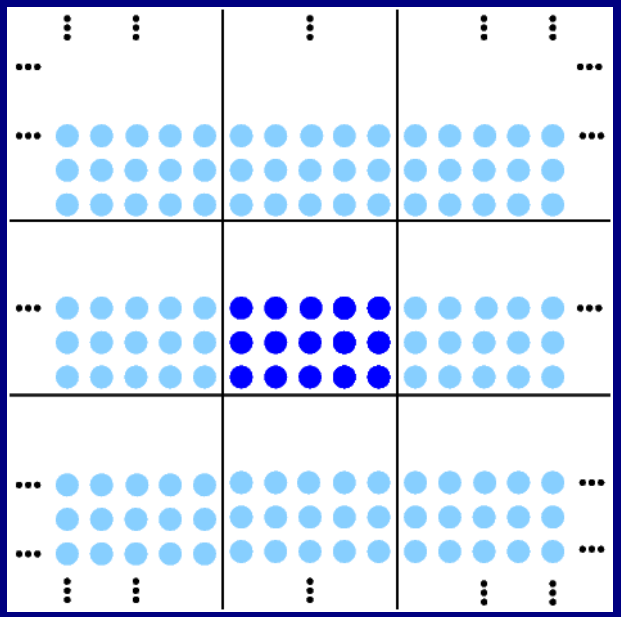
$V_{XC}[n_0](\mathbf{r})$ unknown: local density approximation (LDA)

Density functional theory

after Hohenberg, Kohn and Sham

- using software package VASP for calculations

Supercell:



- pseudopotentals

On SiC: properties

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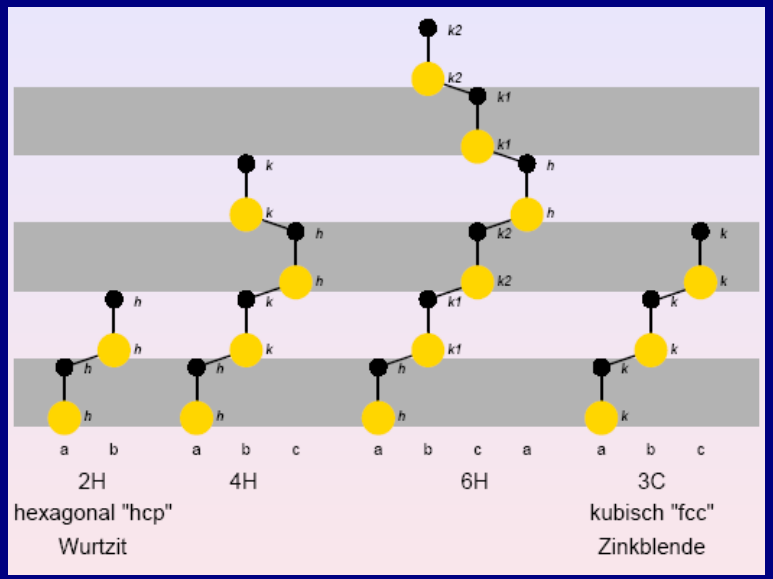
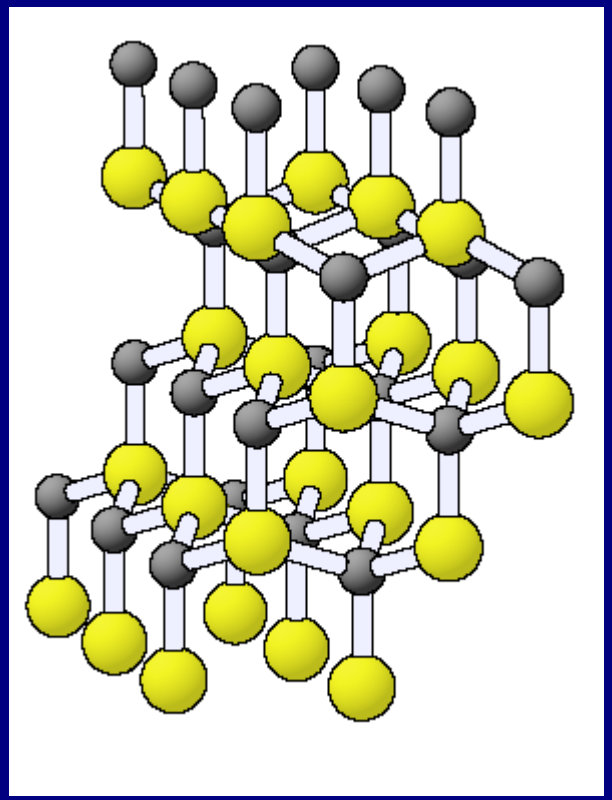
Semiconductor:

- polytypism





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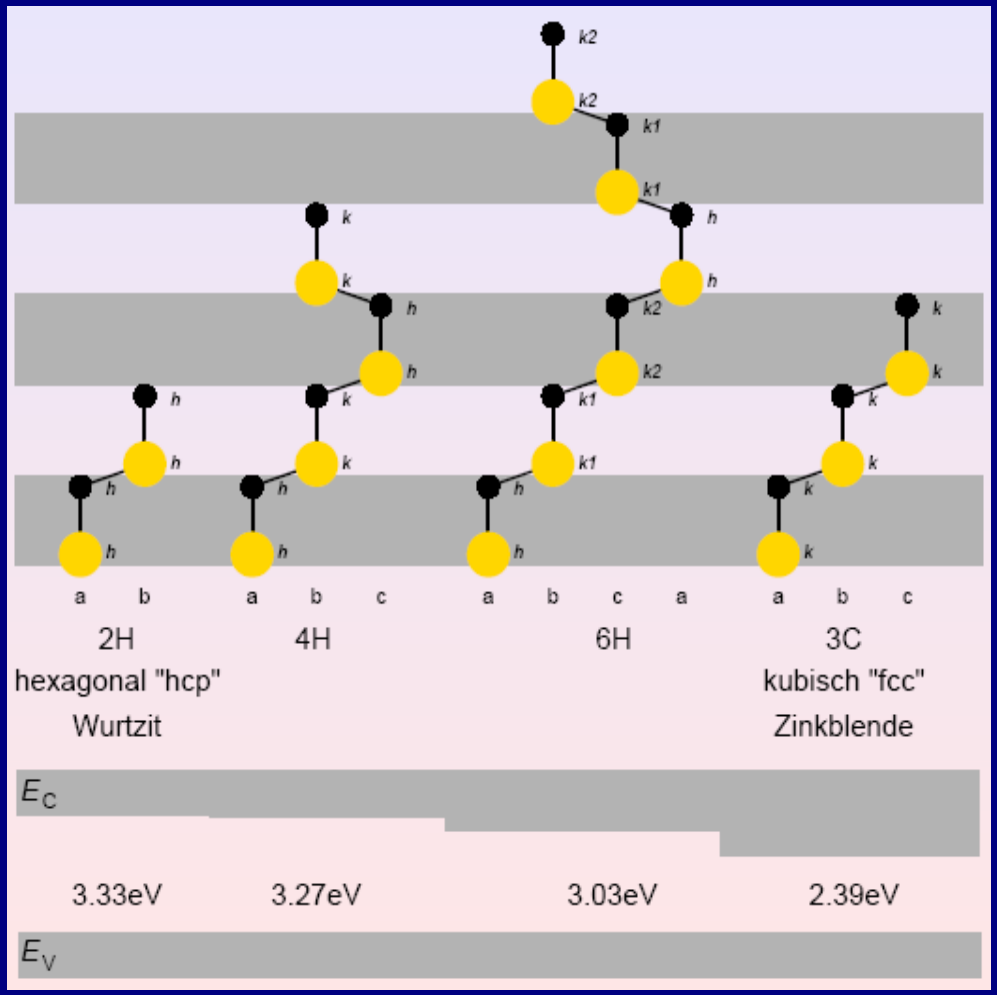
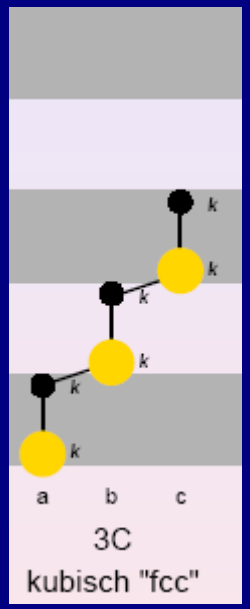


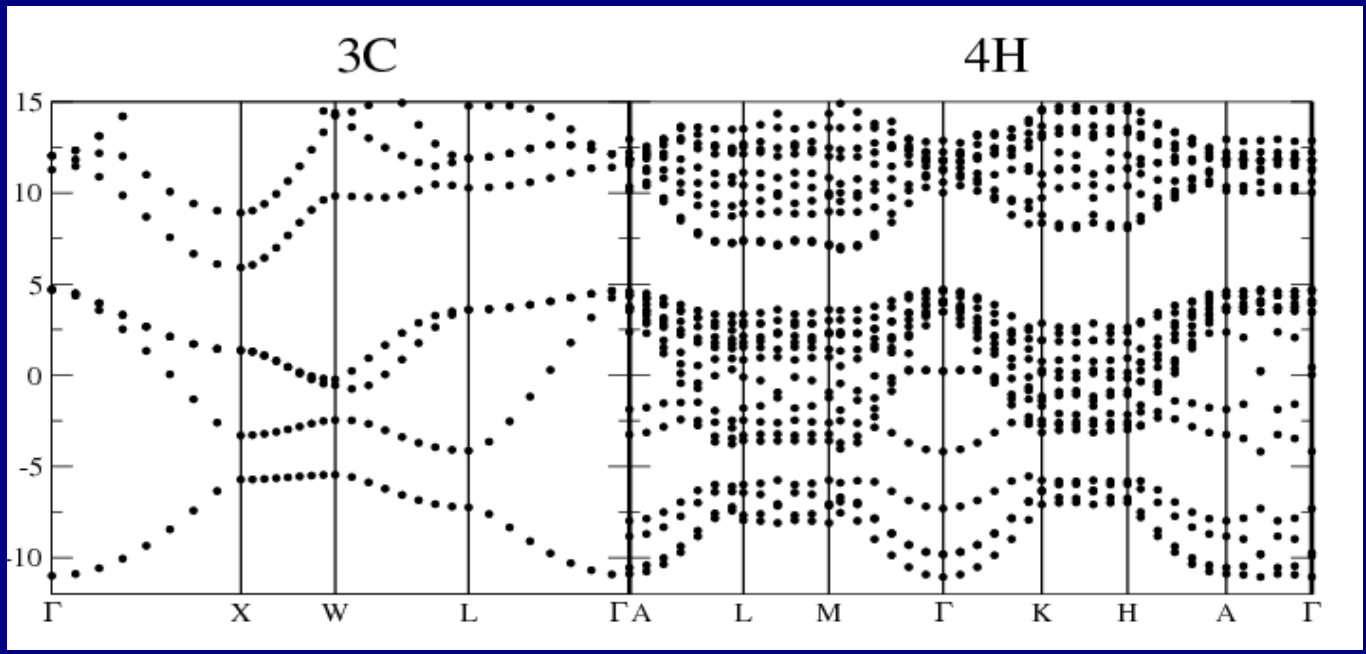
- wide band gap

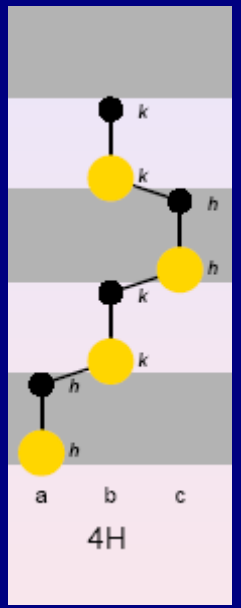
On SiC: properties

Semiconductor:

- Band structure







On SiC: properties

Semiconductor:
- band gap ~ 3 eV
- high electron saturation velocity
- high thermal, mechanical and chemical stability

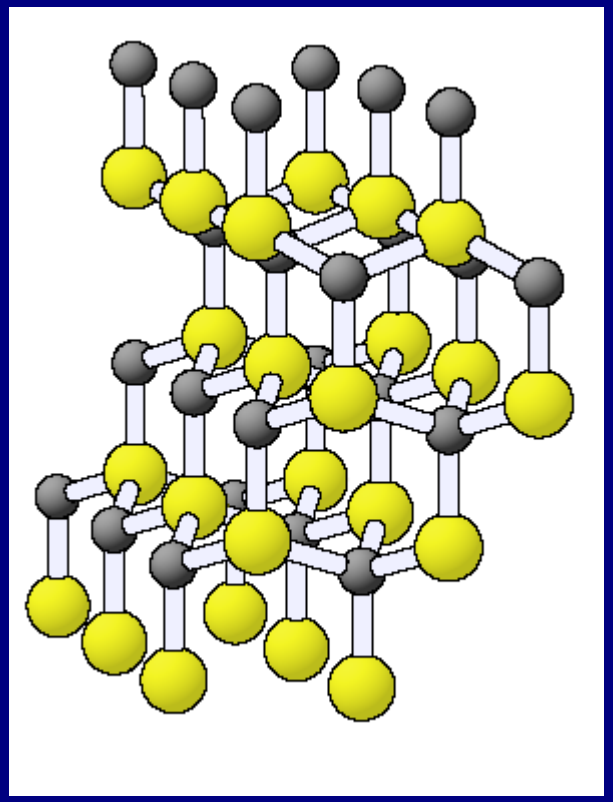
- high-temperature,
- high-frequency,
- and high-power

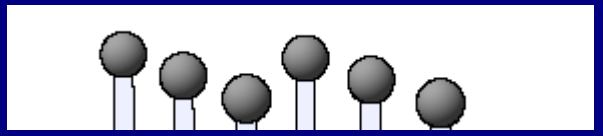
Semiconductor devices

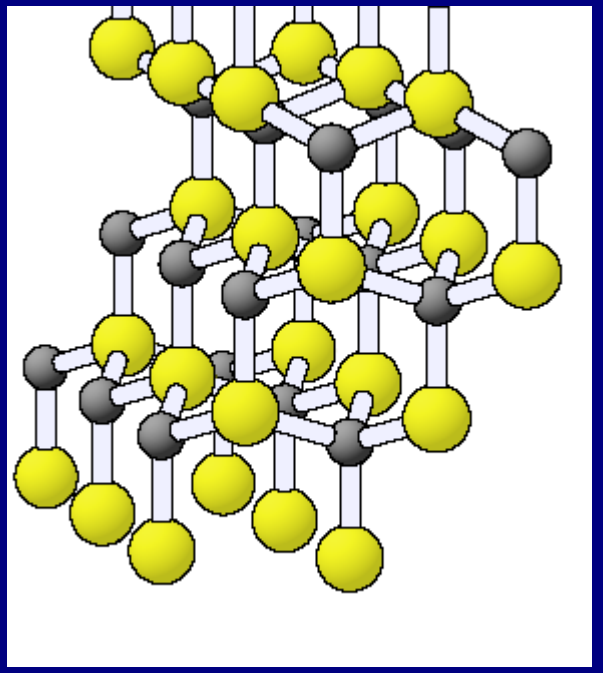
On SiC: surface reconstructions

rearrangment of atoms at a surface

On SiC: surface reconstructions







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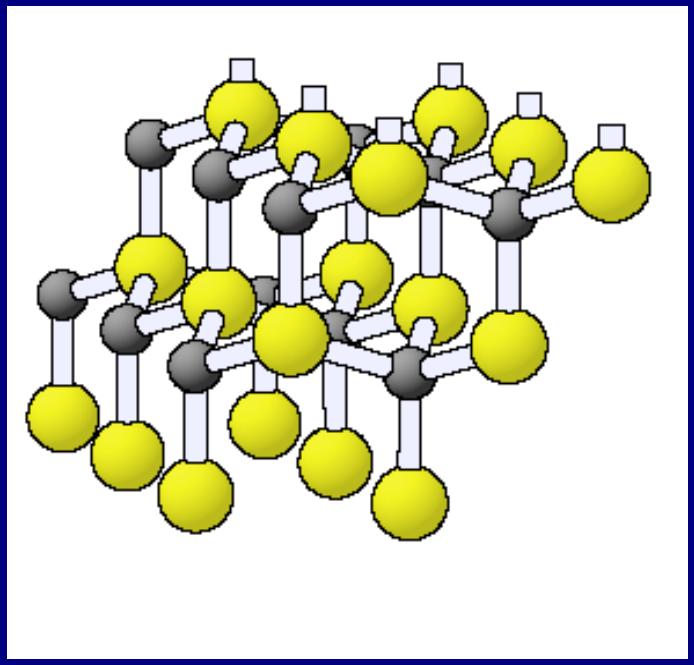

unreconstucted SiC (0001)

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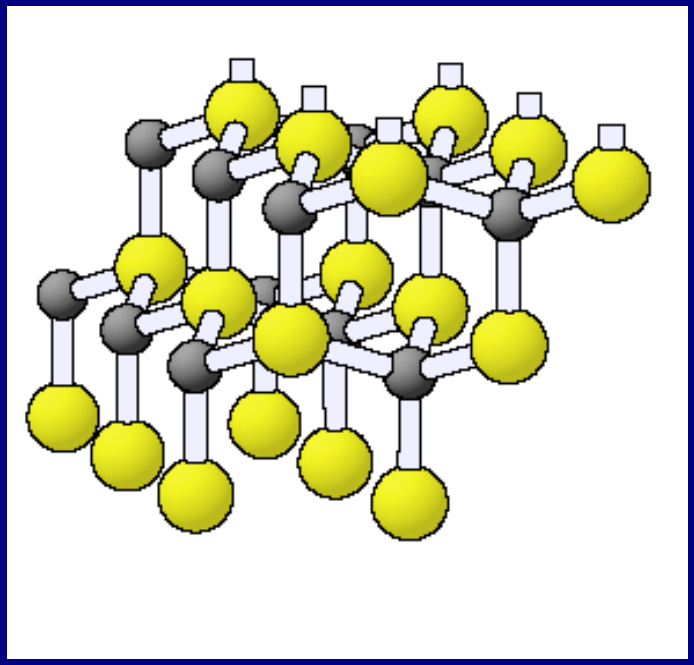

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What happens at the surface?

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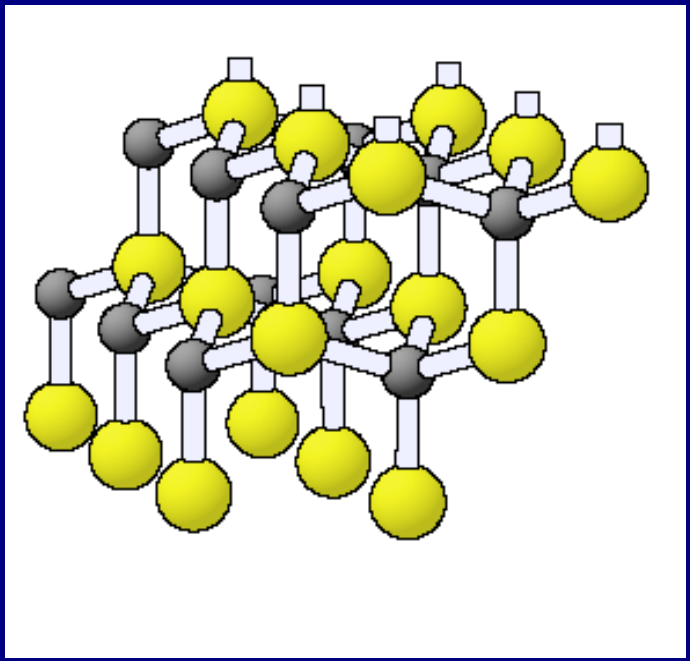

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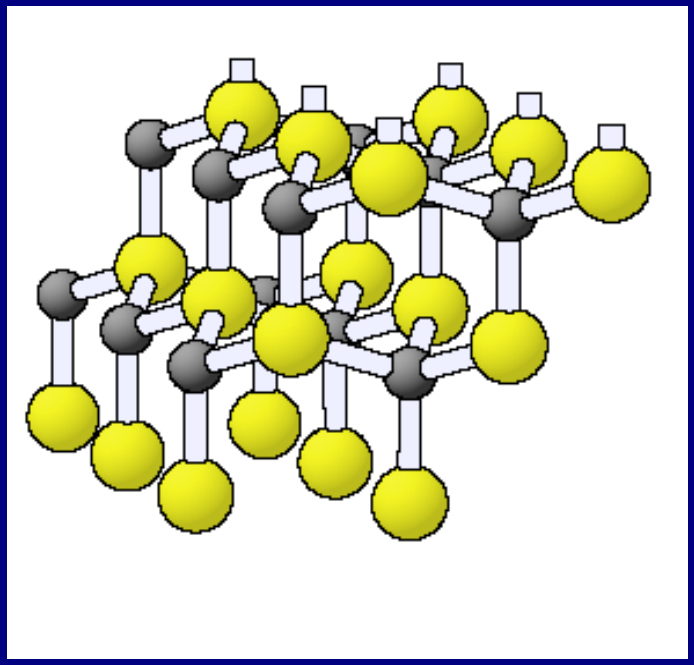
What happens at the surface?

Interaction of the dangling bonds: bond saturation

On SiC: surface reconstructions



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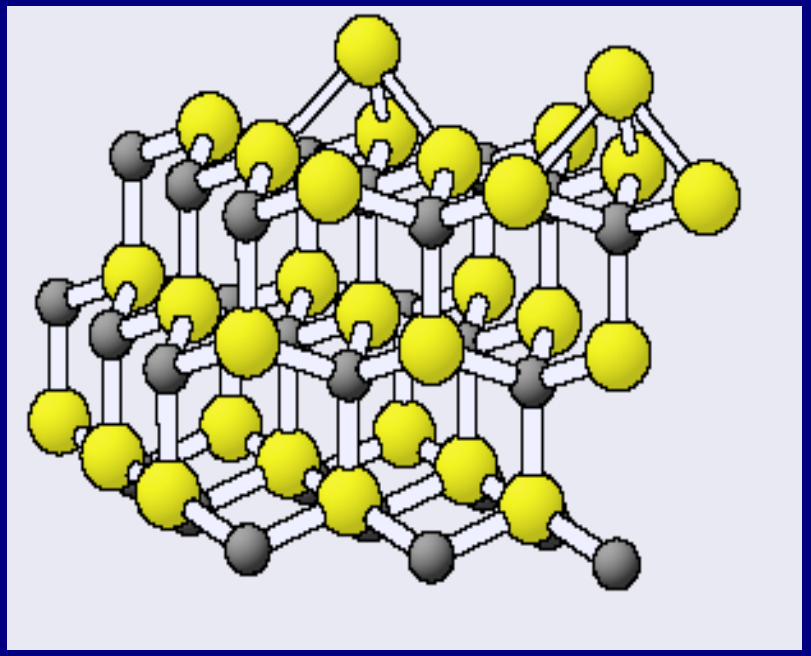
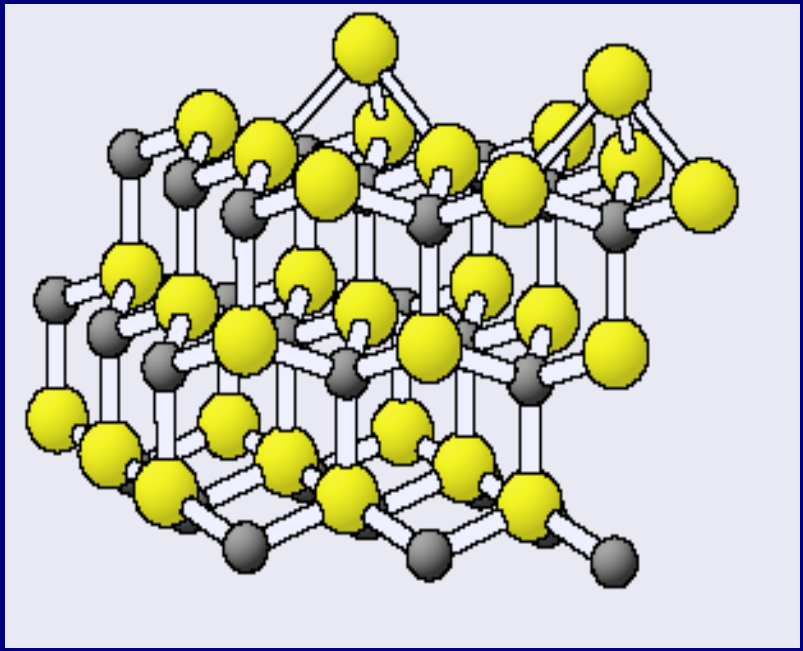
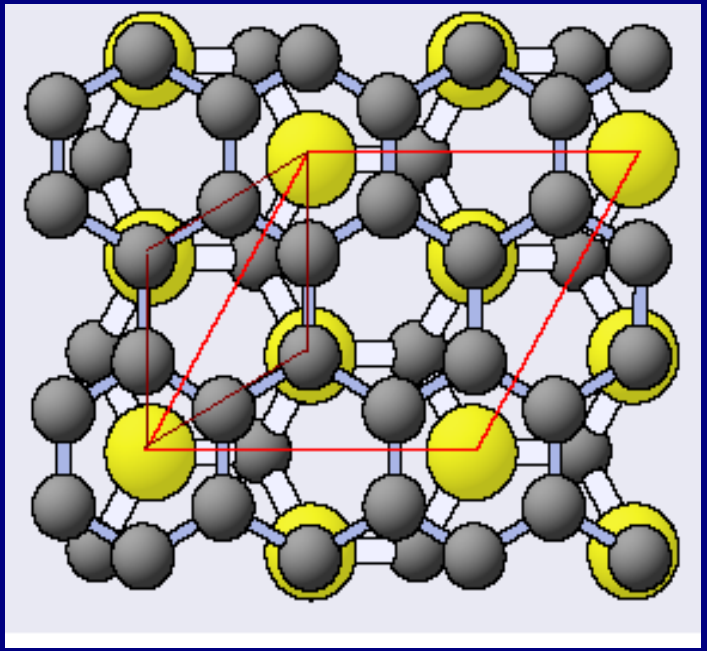


$SiC(0001)\text{-}\sqrt{3} \times \sqrt{3}R30^\circ$

reconstucted SiC:
- silicon-rich with Si adatoms
- 30° rotated unit cell

On SiC: reconstructions





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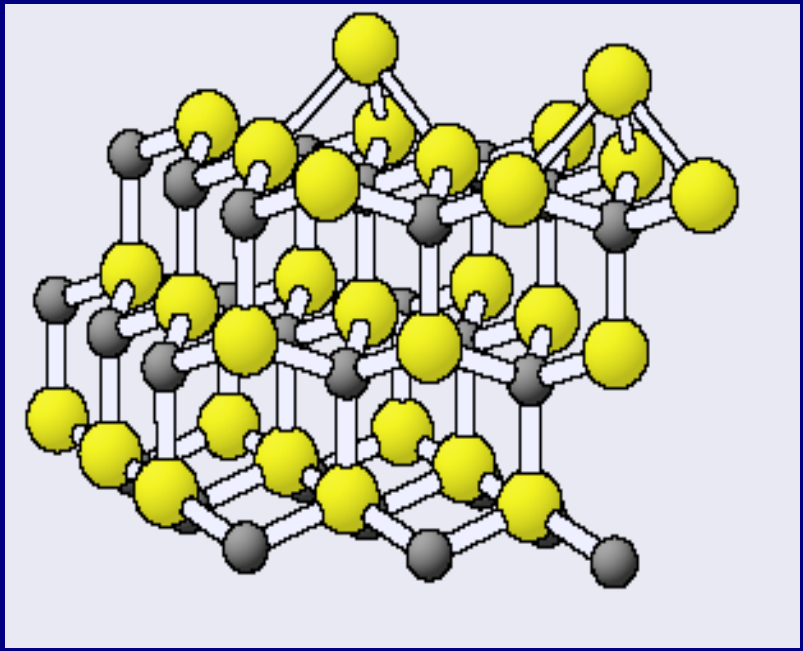

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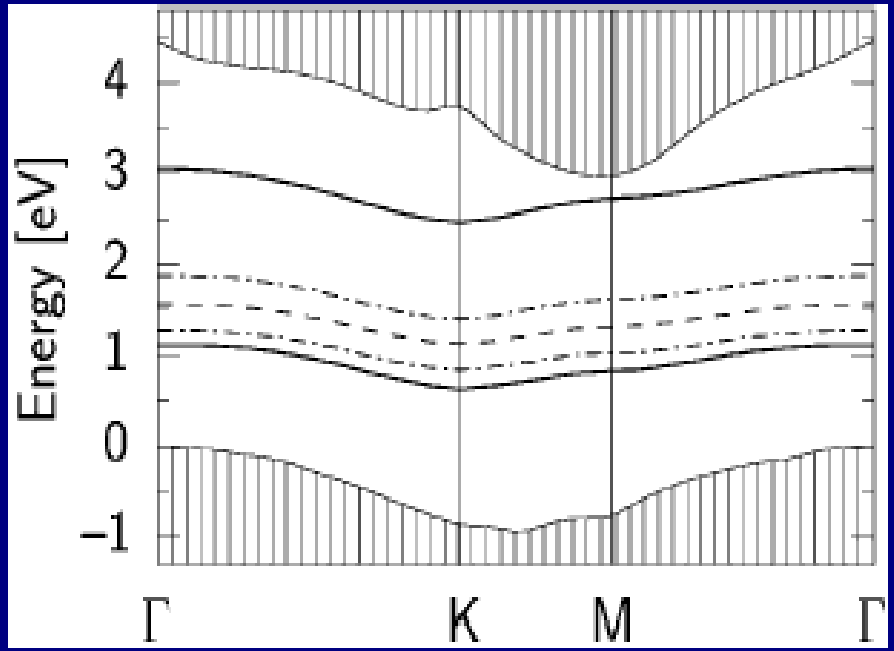

Band stucture

On SiC: surface reconstructions

Hubbard-Mott system
necessary prior conditions:

- low interaction between neighbour orbitals
- strong self-interaction (Hubbard parameter U)

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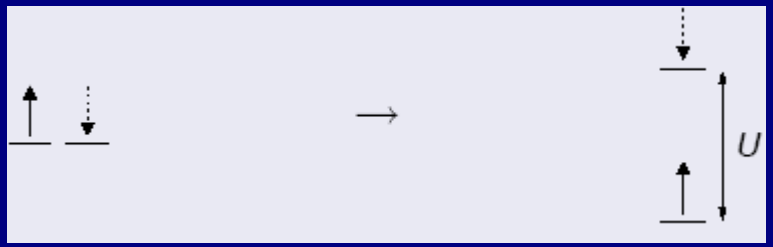
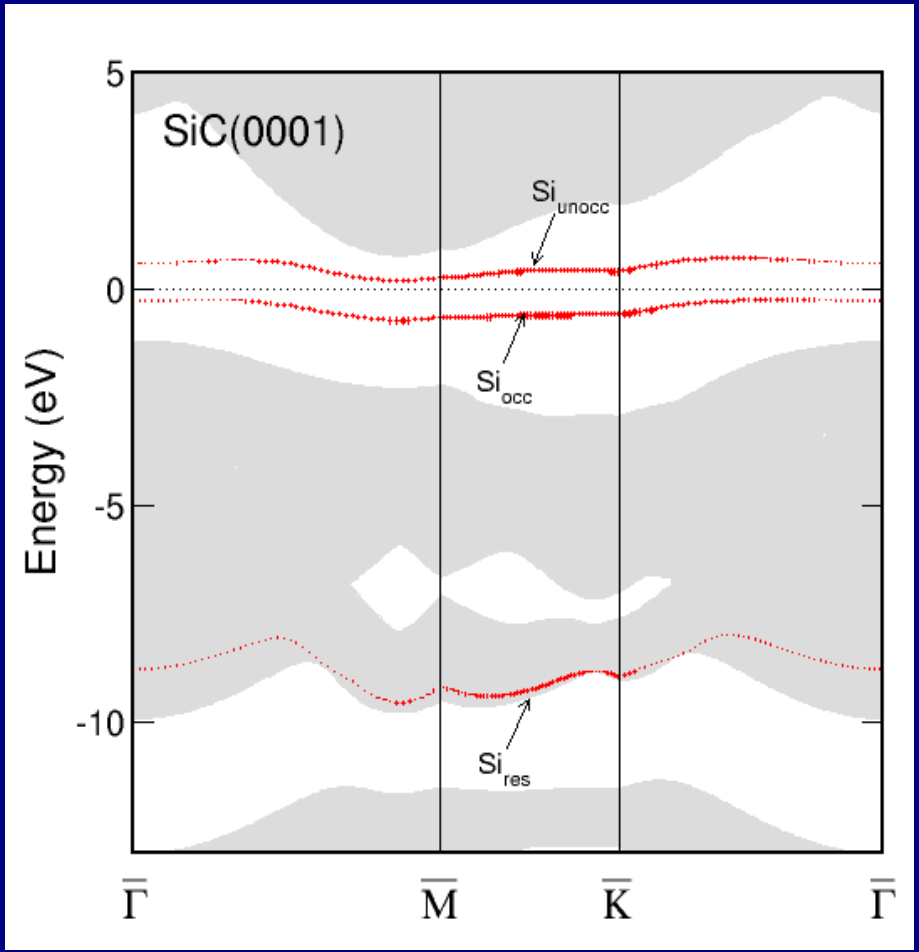
Effects on the band structure:

$$\epsilon_{1,2}(\mathbf{k}) \rightarrow \begin{array}{c} \epsilon_1(\mathbf{k}) = \epsilon_0 + \epsilon(\mathbf{k}) \\ \epsilon_2(\mathbf{k}) = \epsilon_0 + \epsilon(\mathbf{k}) + U \end{array}$$



On SiC: surface reconstructions

Band structure of 1 x 1 SiC:



Production of SiC/Graphene

Annealing at elevated temperatures under vacuum

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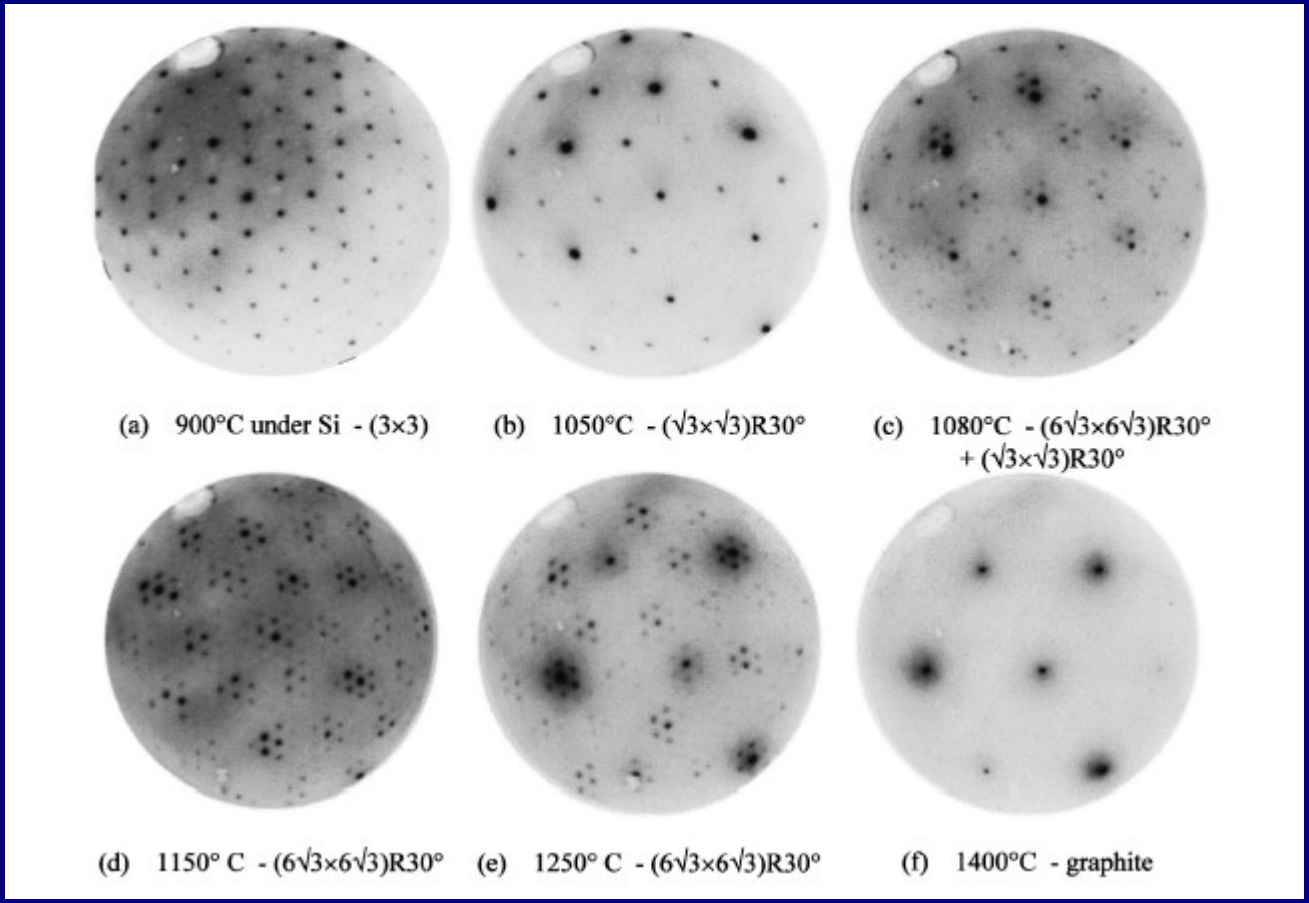

LEED patterns from *6H*-SiC (0001)

Production of SiC/Graphene

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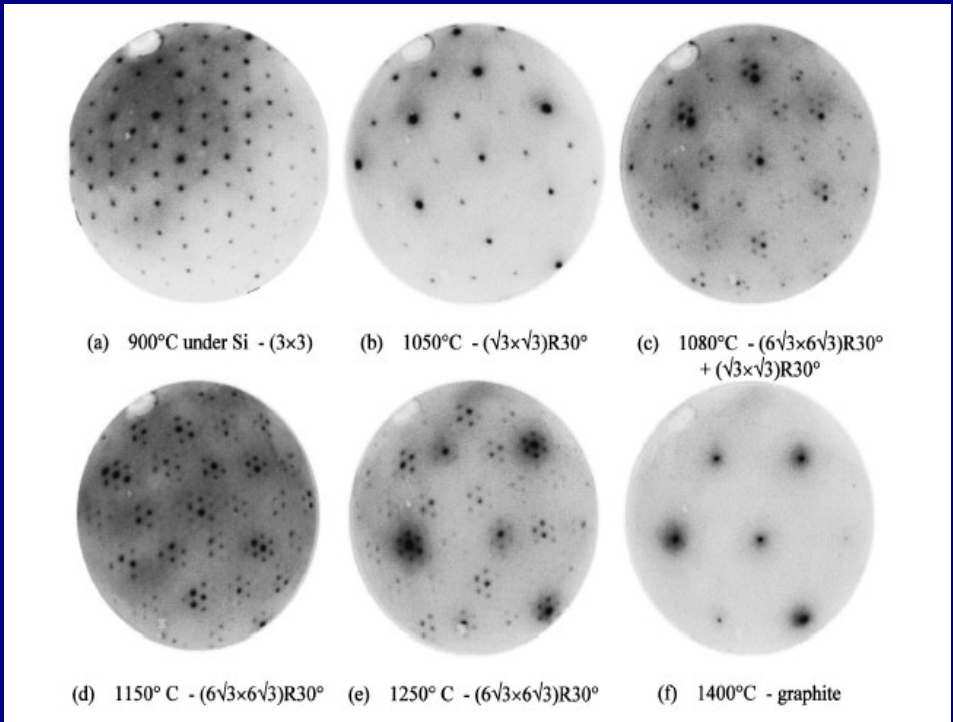
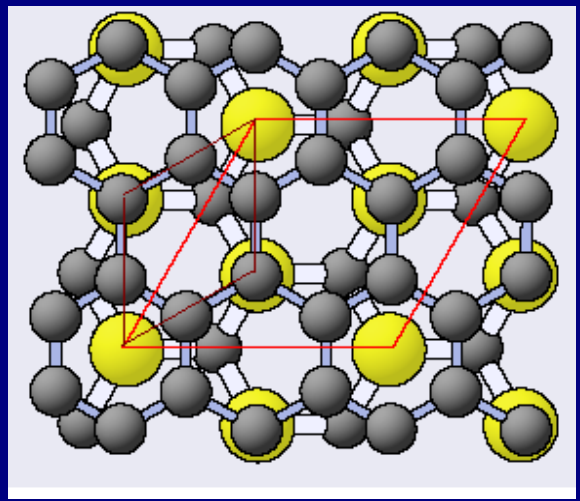


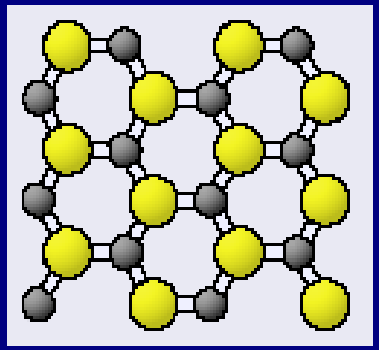


LEED patterns from *6H*-SiC (0001)

(b) $\sqrt{3} \times \sqrt{3}R30^{\circ}$

model interface

Substrate:
unreconstructed 1 × 1-6H-SiC(0001)



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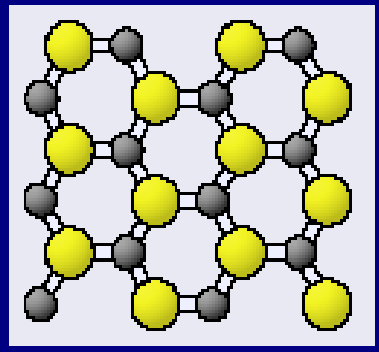
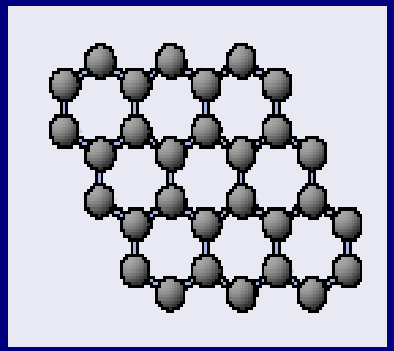


Graphene layer rotated by 30 and stretched by 8%



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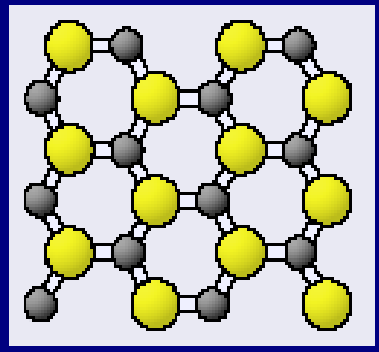
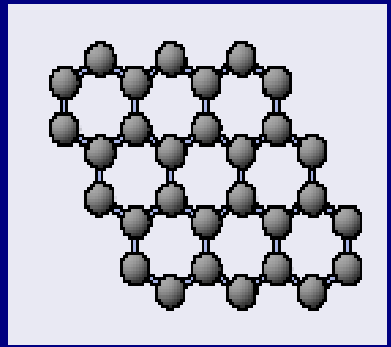


Graphene layer rotated by 30 and stretched by 8%

- stretch reduces total bandwidth (19,1eV→17.3eV)
- electronic spectrum close to Fermi energy unchanged
- elastic energy 0.8eV per graphene unit cell



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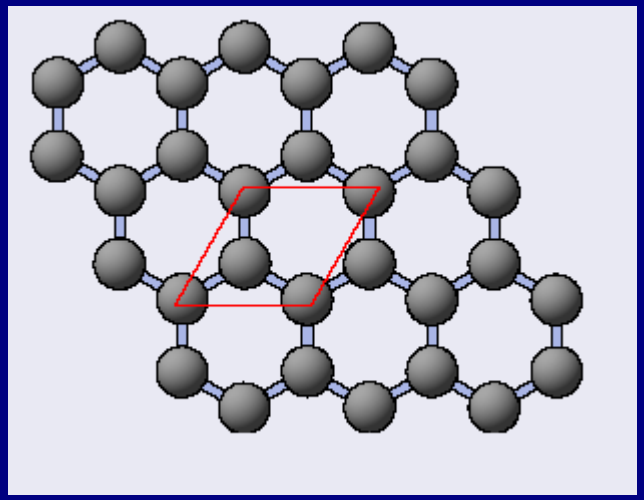
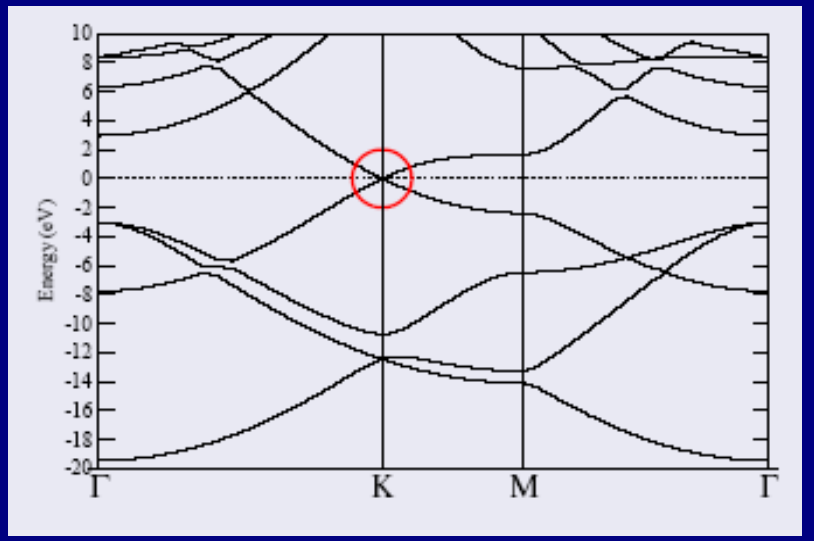


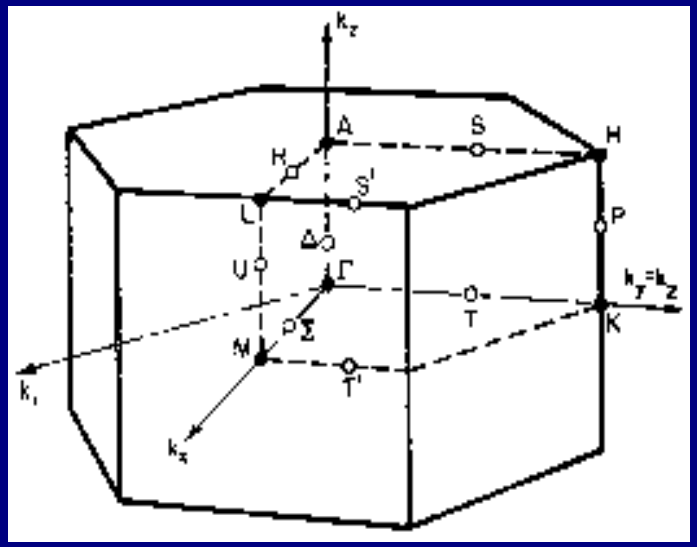
Atomic structure



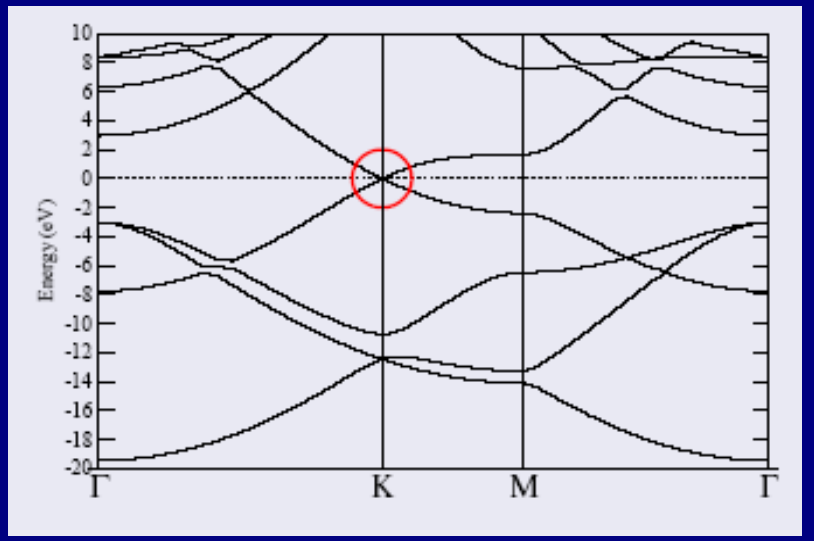
Band Stucture:

- conic point at $\bar{K}$
- semi-metal

Graphene



Brillouinzone



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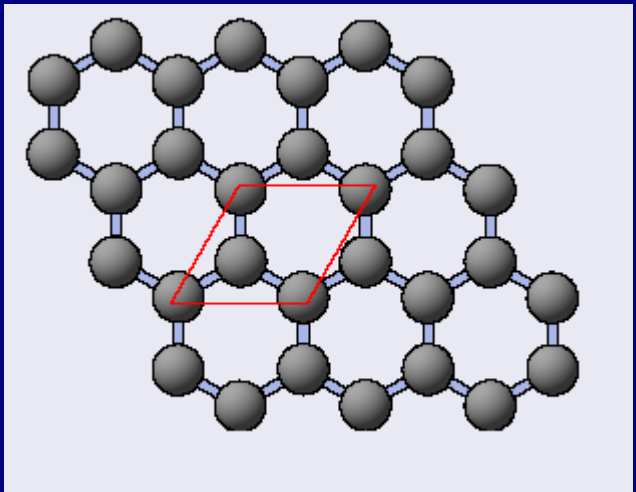

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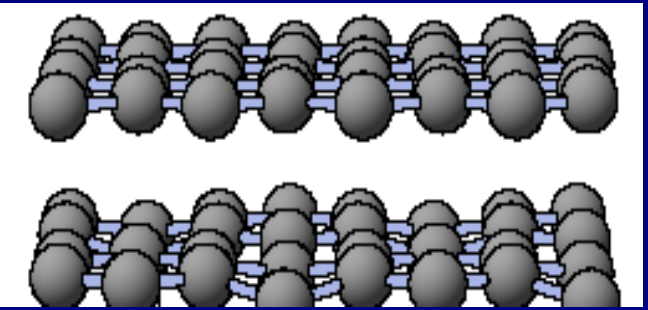
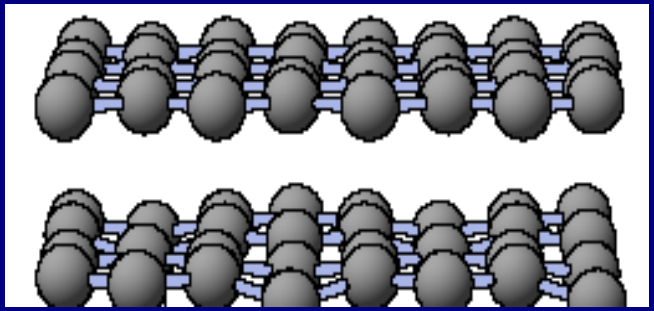


graphene layers bound by van der Waals forces

Graphene



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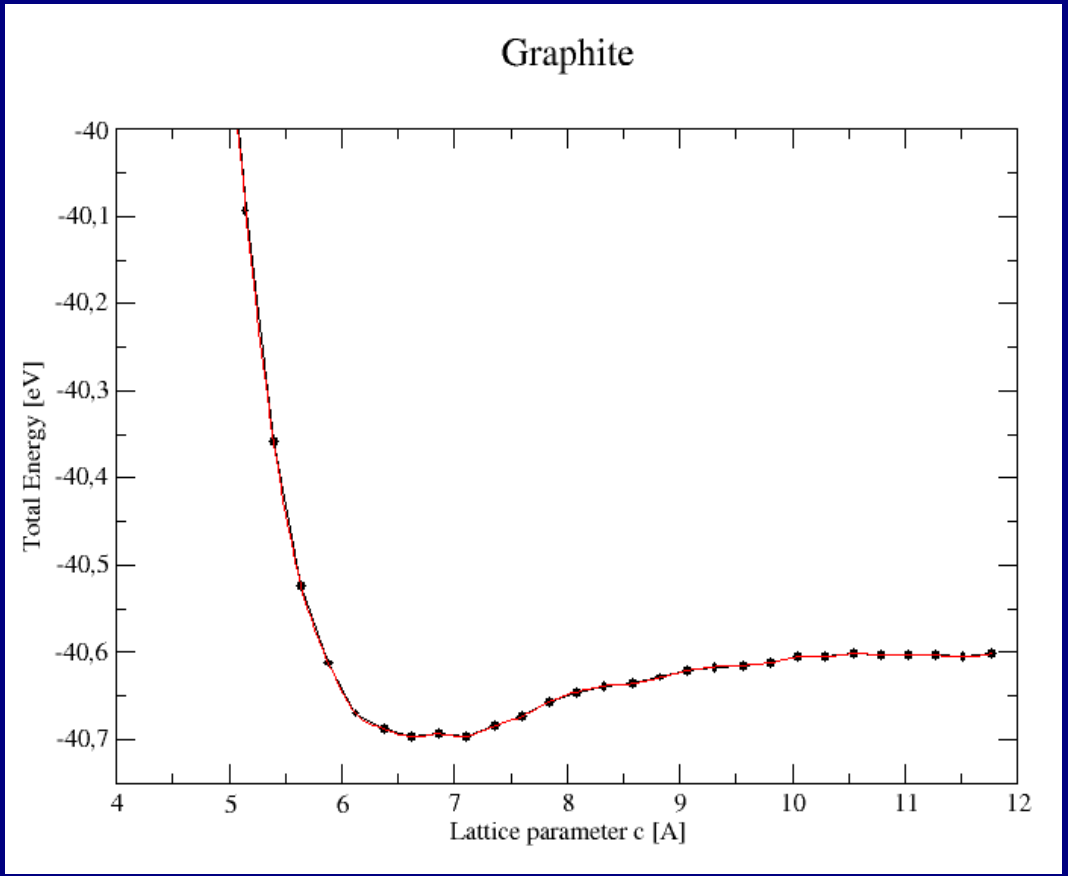
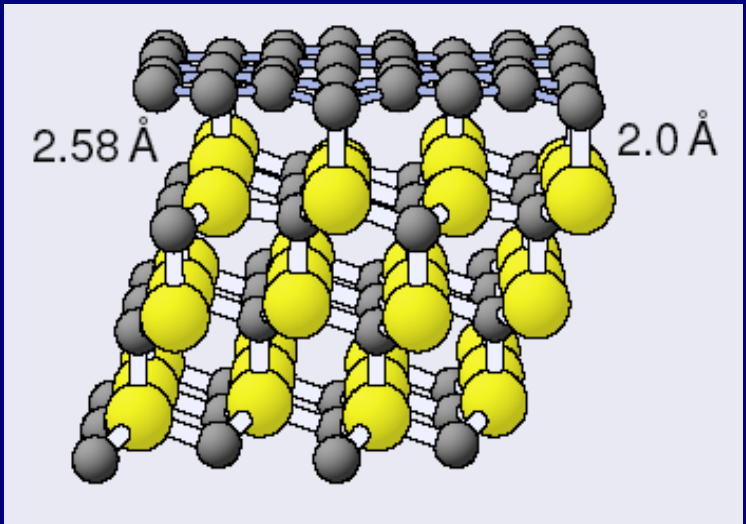


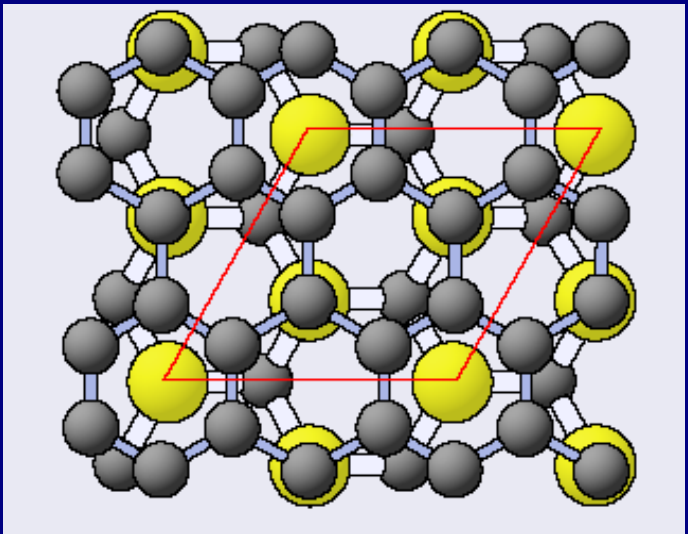
Results of the calculations

Results of the calculations

SiC(0001)/ Graphene:



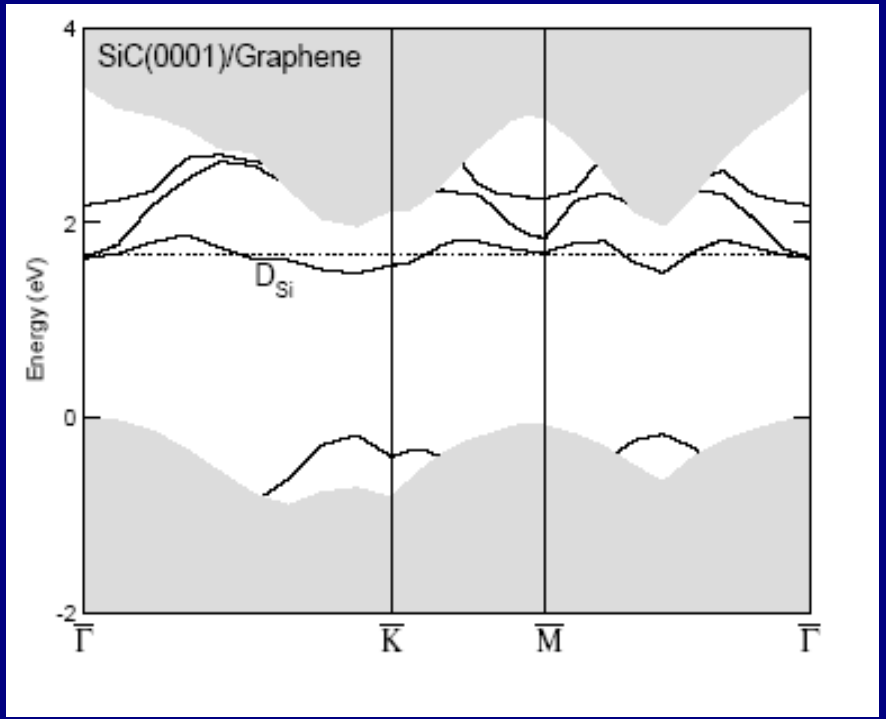
Graphene on 1 × 1-SiC(0001)
Side view



Graphene on 1 × 1-SiC(0001)
Top view

Results of the calculations

SiC(0001)/ Graphene:
Band structure:

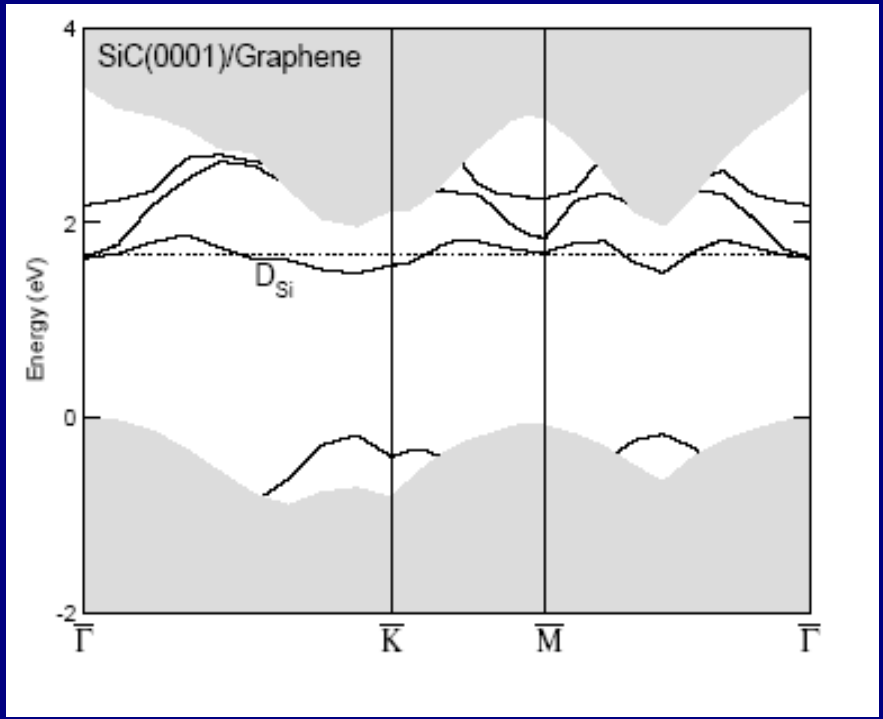


Results of the calculations

SiC(0001)/ Graphene:
Band structure:

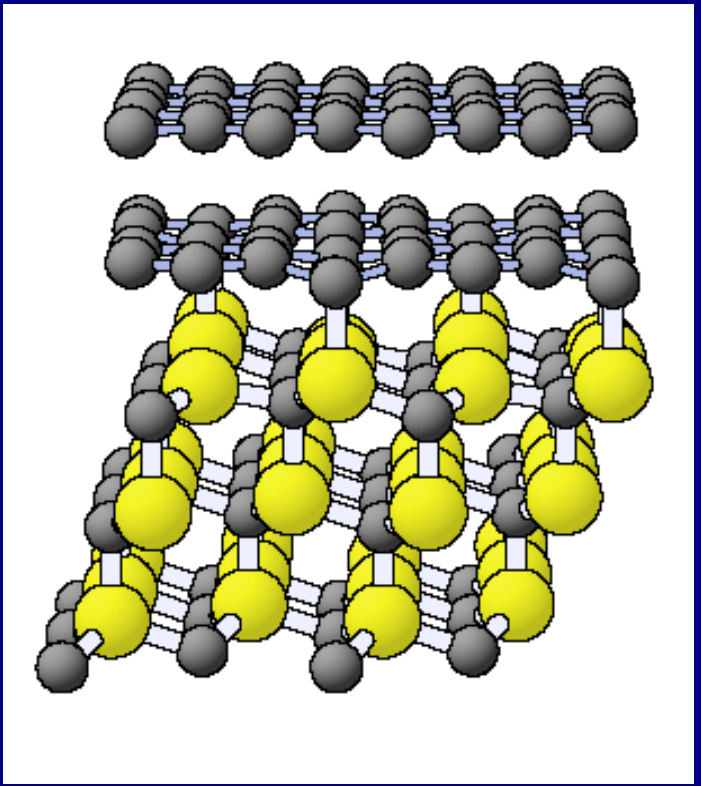
- D_{si}: interface state
- metallic
- mixture of dangling bond and graphene
- Fermi-Level pinned:

→strong band bending



Results of the calculations

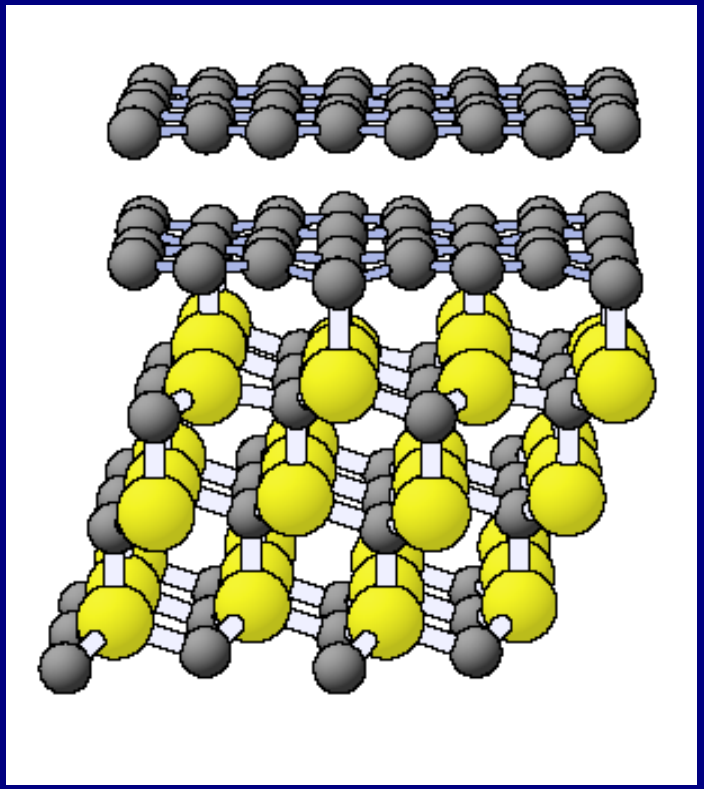
SiC(0001)/2 layers Graphene:



Results of the calculations

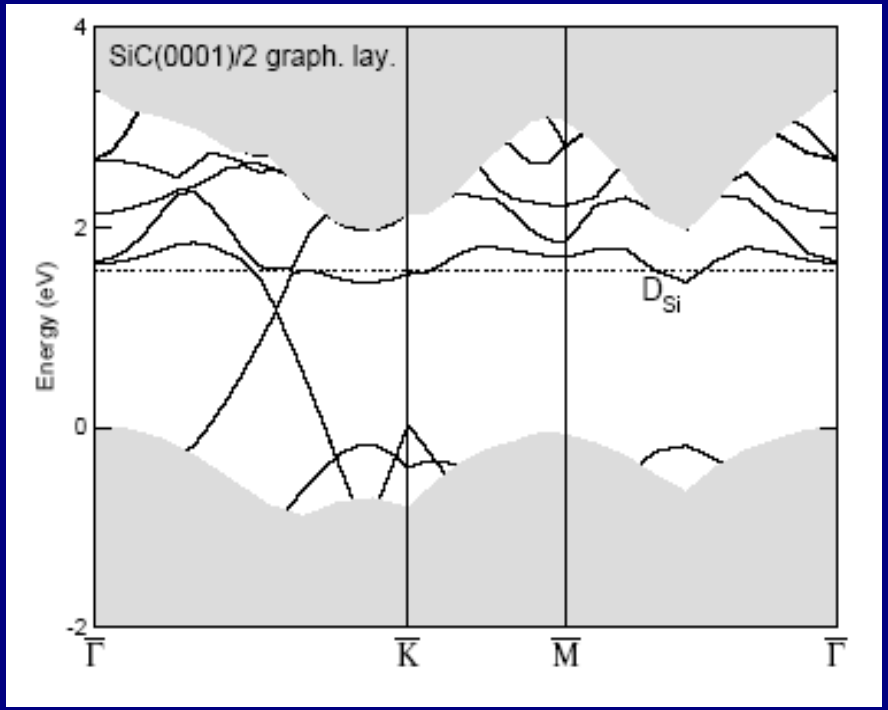
SiC(0001)/2 layers Graphene:

- 1st layer: covalently bonded
- 2nd layer: only van der Waals forces



Results of the calculations

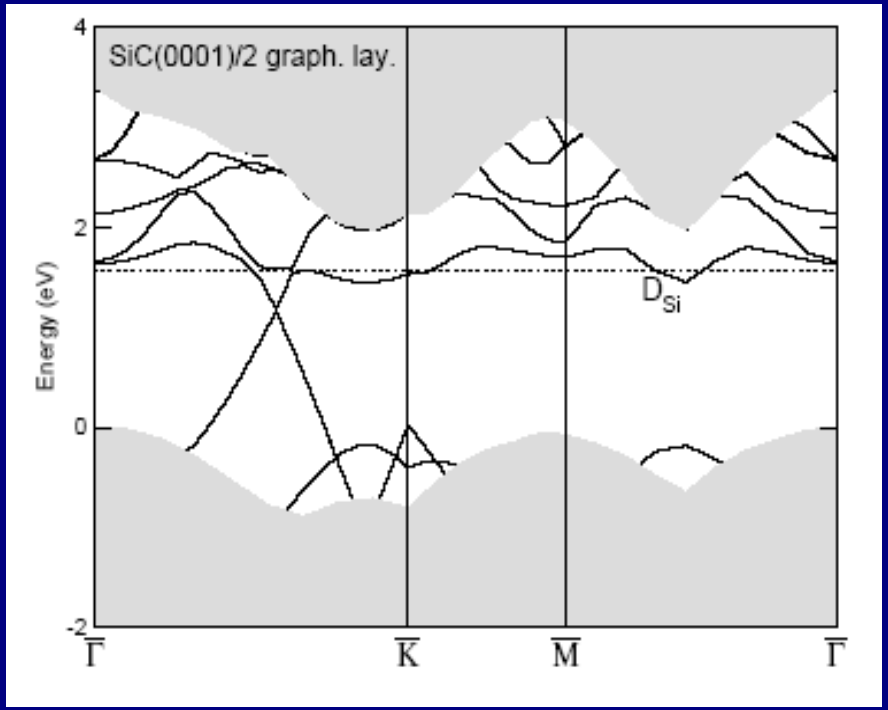
SiC(0001)/2 layers Graphene:
Band structure:



Results of the calculations

SiC(0001)/2 layers Graphene:
Band structure:

- Fermi-Level still pinned
  → charge flow to graphene
- Conic point appears below E_F
- further graphitic states



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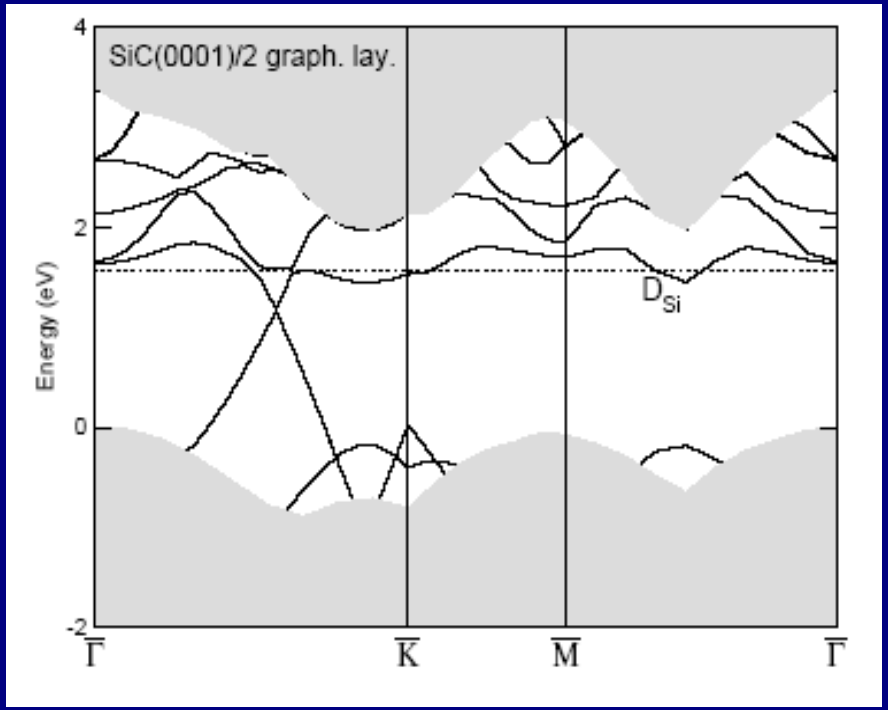
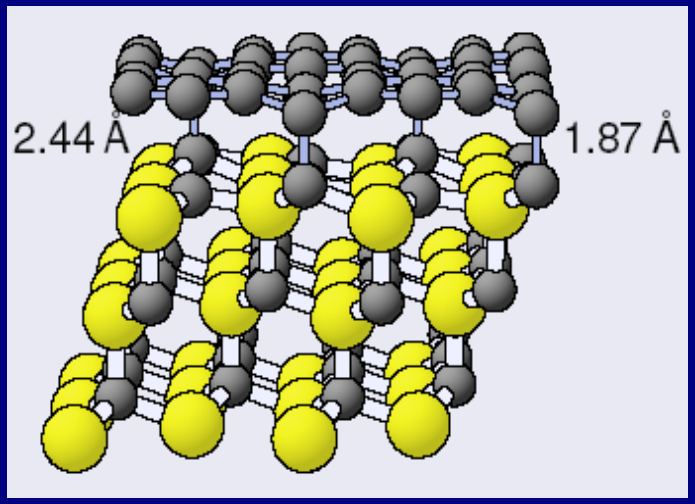


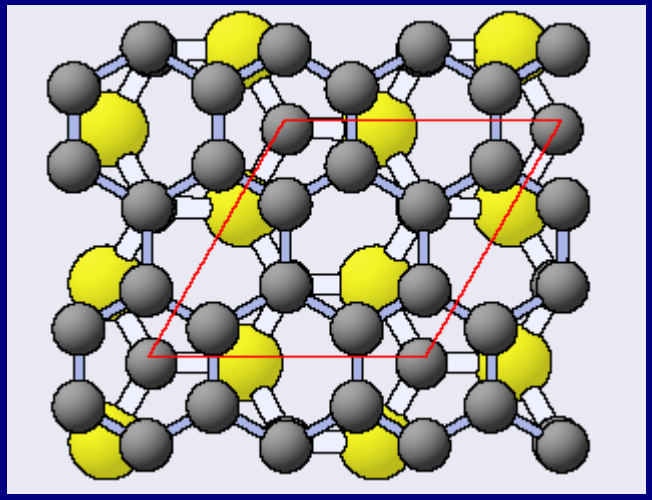
still metallic interface,
no splitting of the interface state D_{Si}

Results of the calculations

Graphene on 1 × 1-SiC(000-1):



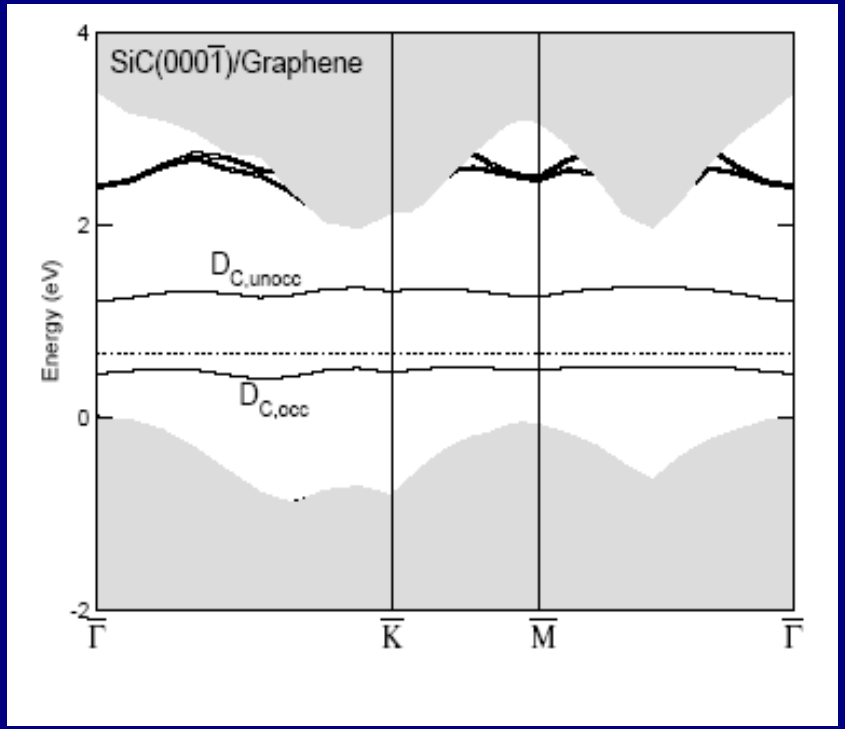
Graphene on 1 × 1-SiC(000-1)
Side view



Graphene on 1 × 1-SiC(000-1)
Top view

Results of the calculations

Graphene on 1 × 1-SiC(000-1):
Band structure:

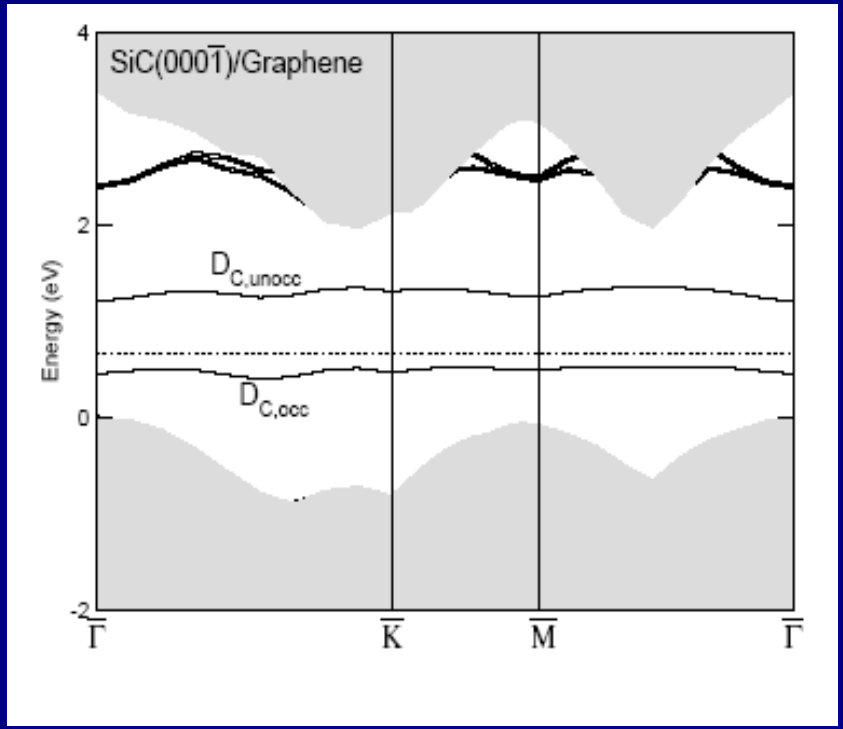


Results of the calculations

Graphene on 1 × 1-SiC(000-1):
Band structure:

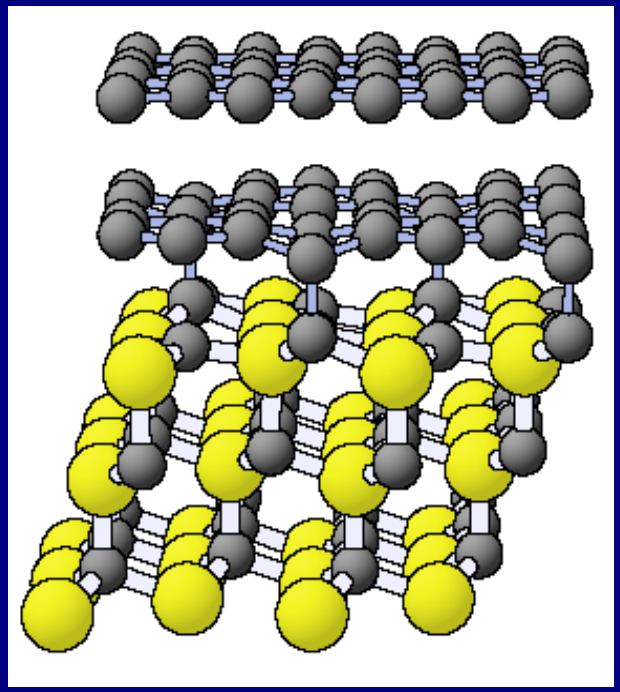
- C-dangling bond does not interact with the graphene layer
- D_C splits (selfinteraction)

→ semiconducting interface



Results of the calculations

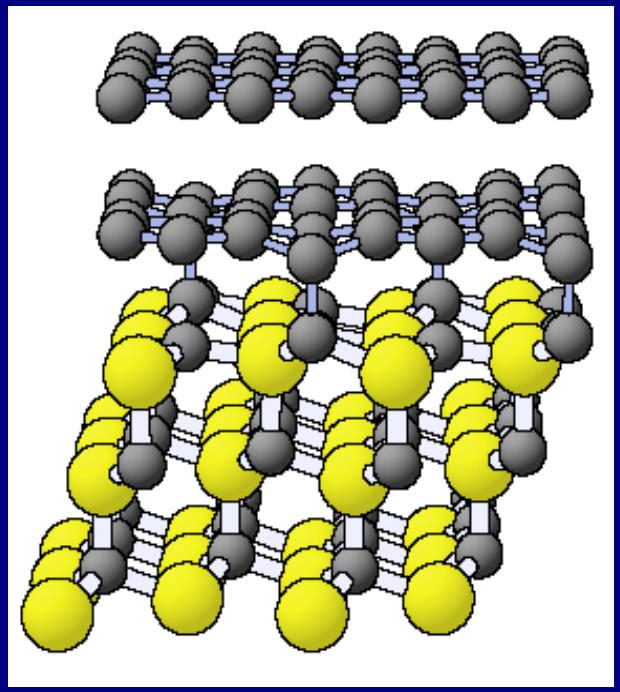
SiC(000-1)/2 layers Graphene:



Results of the calculations

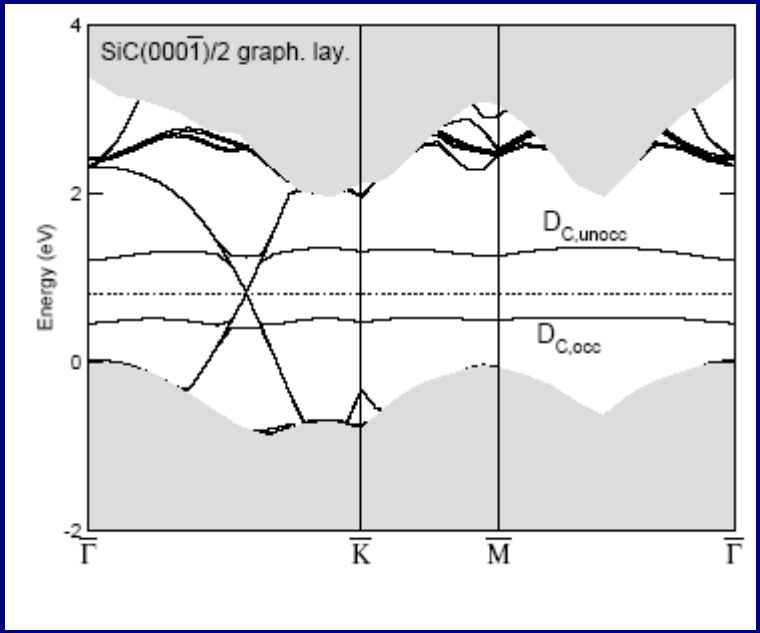
SiC(000-1)/2 layers Graphene:

- 1st layer: covalently bonded
- 2nd layer: weak bonded



Results of the calculations

SiC(000-1)/2 layers Graphene:
Band structure:

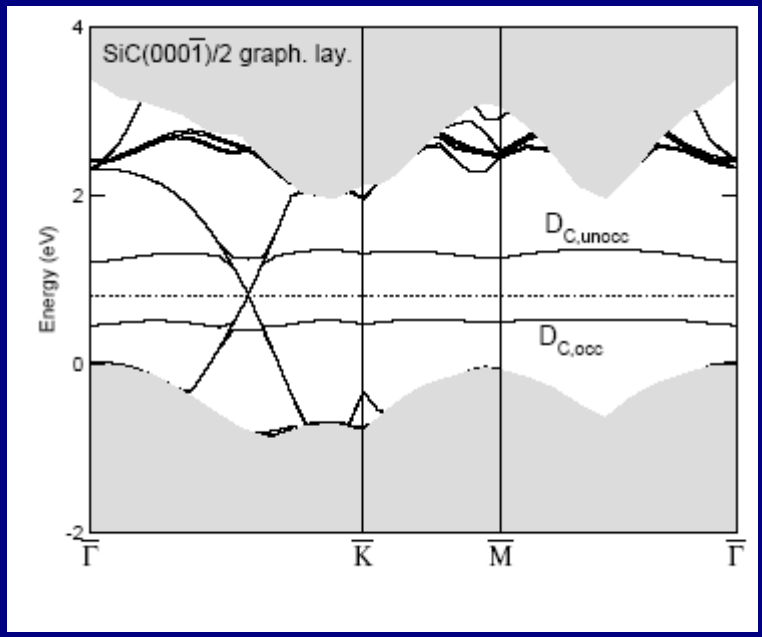


Results of the calculations

SiC(000^{-}1)/2 layers Graphene:
Band structure:

- conic point
- Fermi-Level determined by graphene

→ semimetallic behaviour



Results of the calculations

Comparision of both sides: SiC(0001)/Graphene and SiC(000-1)/Graphene

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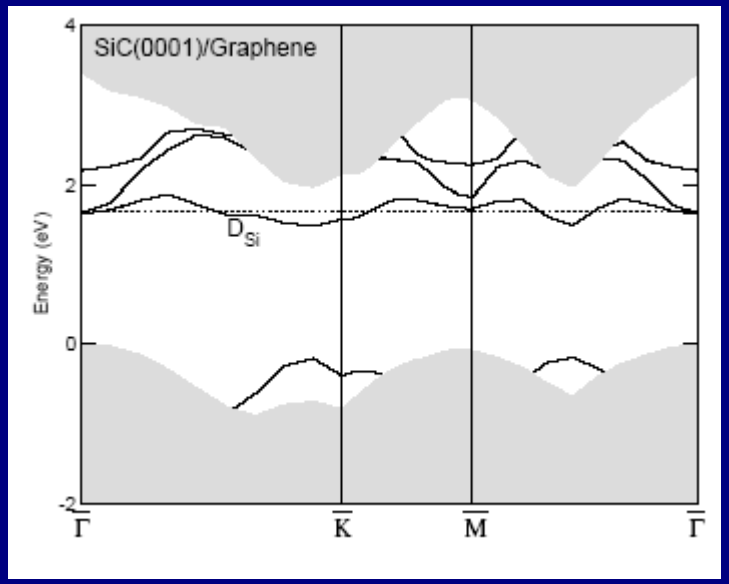
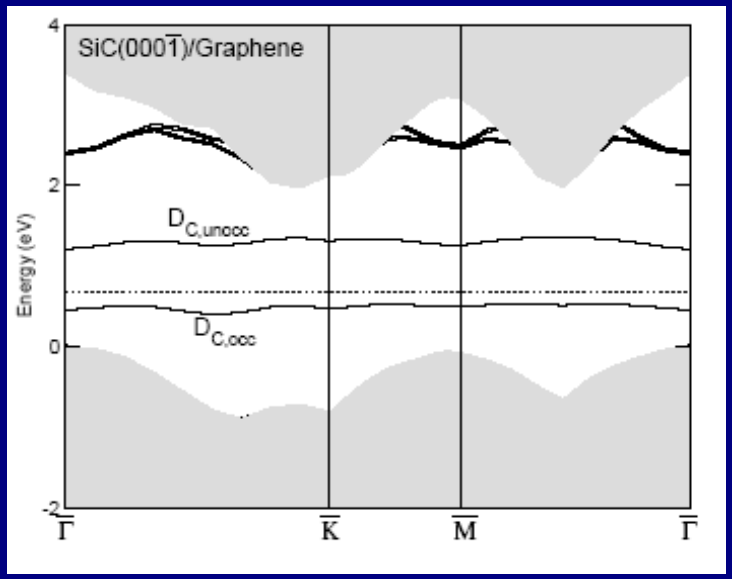
Band structures:





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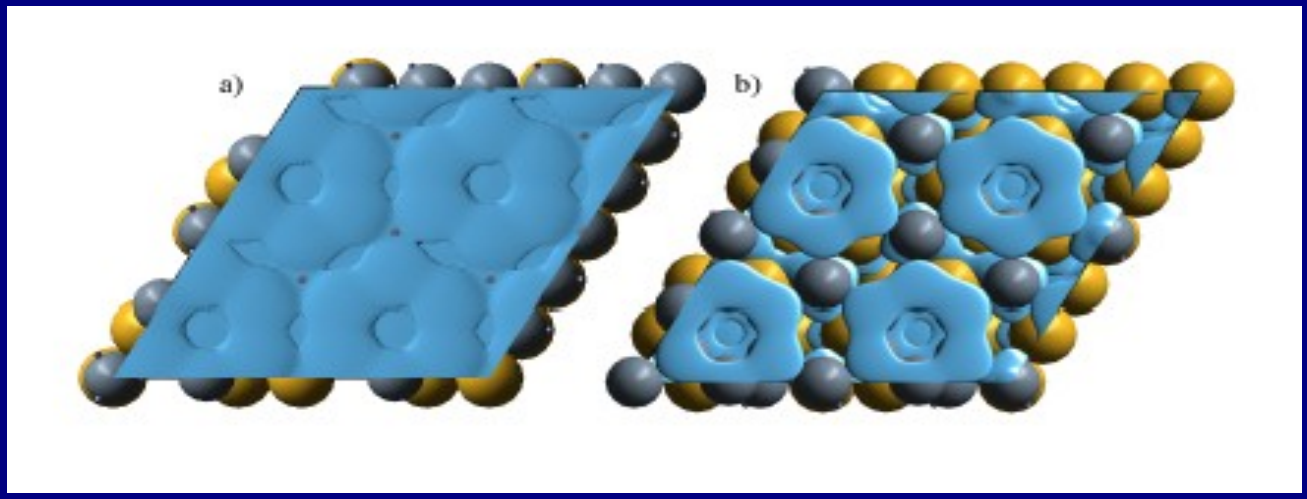
Charge density of the interface states at Fermi energy:



a) SiC(0001)

b) SiC(000-1)

Results of the calculations

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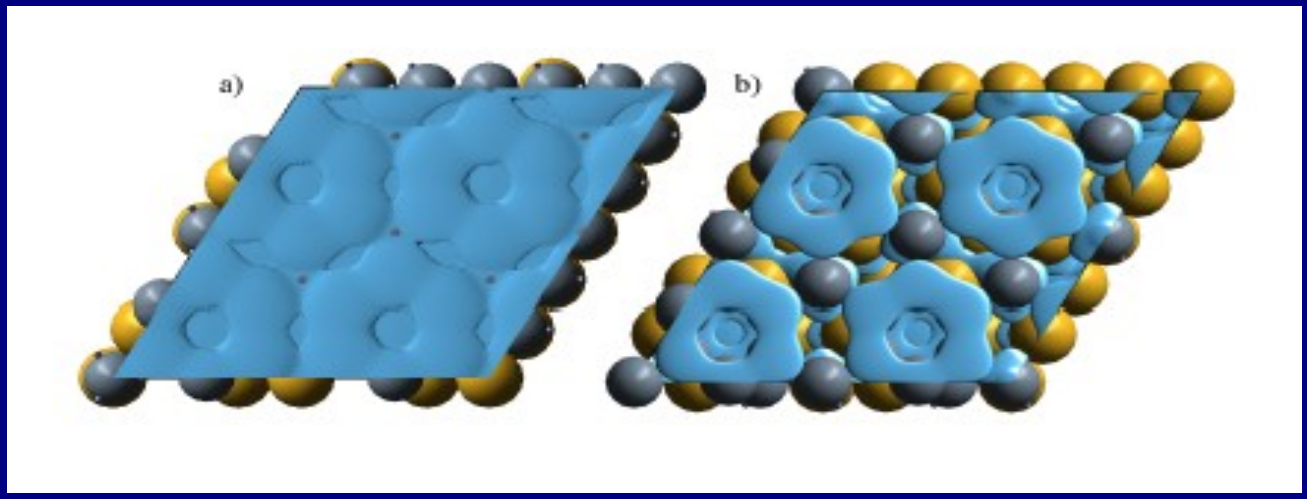

a) SiC(0001) b) SiC(000-1)

localisation favors spin polarization → splitting of the gap state at b)

Outlook

Outlook

What is still to study:

- Microscopic structure of the interface reconstructions
- Differences between the sides in more detail
  (Experiments on the SiC(000-1) side)

THE END