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Electronic Structures of Two-Dimensional PC_6-type Materials

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Graphene Functionalization To Open Band Gap

- Functionalization of $\sqrt{7} \times \sqrt{7}R19.1°$ super cell of graphene (Fig. 1a, red unit cell) by substitution of marked atoms → PC_6
- PC_6 is a semiconductor with Dirac cones above (green bands) and below (pink bands) the Fermi level (Fig. 1c,d).[1]

➢ How can the Fermi level be shifted to access the Dirac cones?

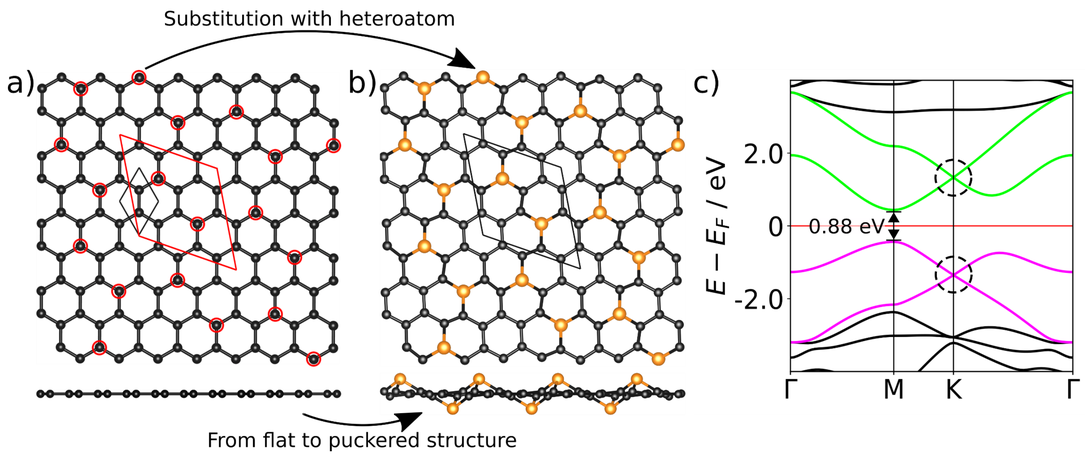

Fig. 1: (a) Graphene monolayer with primitive unit cell (black) and super cell (red), (b) structure of PC_6, (c) band structure of PC_6 with Dirac cones (dashed circles) above (green bands) and below (pink bands) the Fermi level. C black and P orange.

Adatom Strategy

- By adsorption of hydrogen atoms, two electrons are added to the electron filling. This allows to access the Dirac cone above the Fermi level in PC_6.[3]
- Characteristic bands remain the same, since the network structure is not changed.

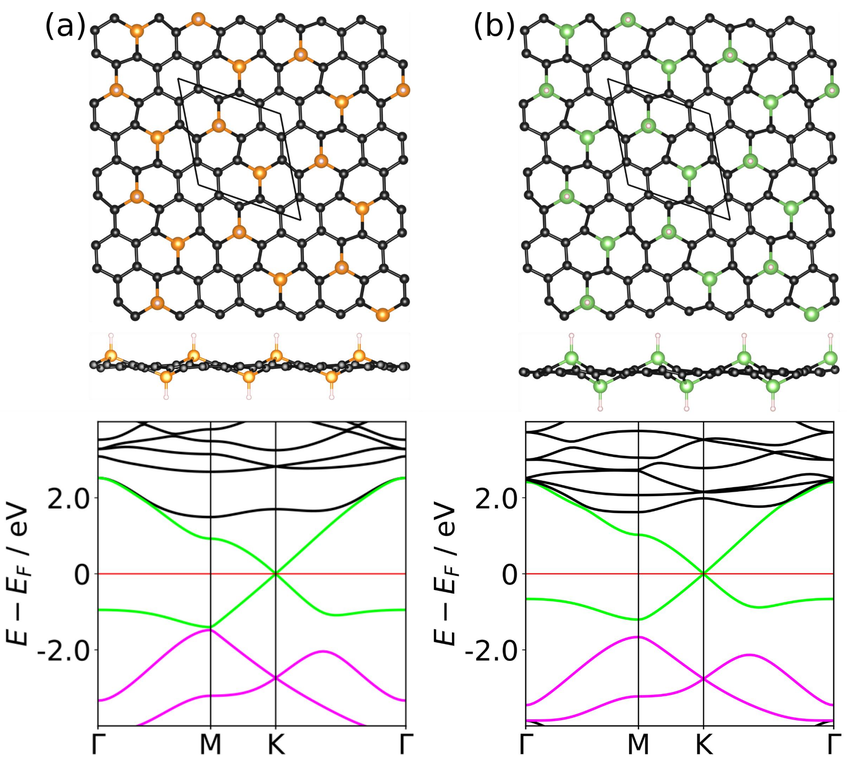

Fig. 3: Structures (top and side view) and band structures of (a) H_2PC_6 and (b) H_2AsC_6. H is white, C is black, P is orange, As is green.

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Substitution Strategy

- If the network structure is retained, also the general shape of the band structure ("characteristic bands") remains the same.
- According to the number of valence atoms, the Fermi level can be shifted to access Dirac cones above and below the Fermi level:
  - Group 14 (Al, Ga): Fermi level below characteristic bands, -4 e^-/cell w.r.t PC_6
  - Group 15 (Ge): Fermi level at lower Dirac cone, -2 e^-/cell w.r.t PC_6.[2]
  - SiC_6: This structure is planar instead of puckered.[2] Therefore, the characteristic bands are shifted downwards and the Fermi level lies at the upper Dirac cone.
  - Group 16 (P, As): Semiconductor with direct band gap at M, Dirac cones above and below Fermi level.
  - Group 17 (S, Se): Fermi level at upper Dirac cone, +2 e^-/cell w.r.t PC_6

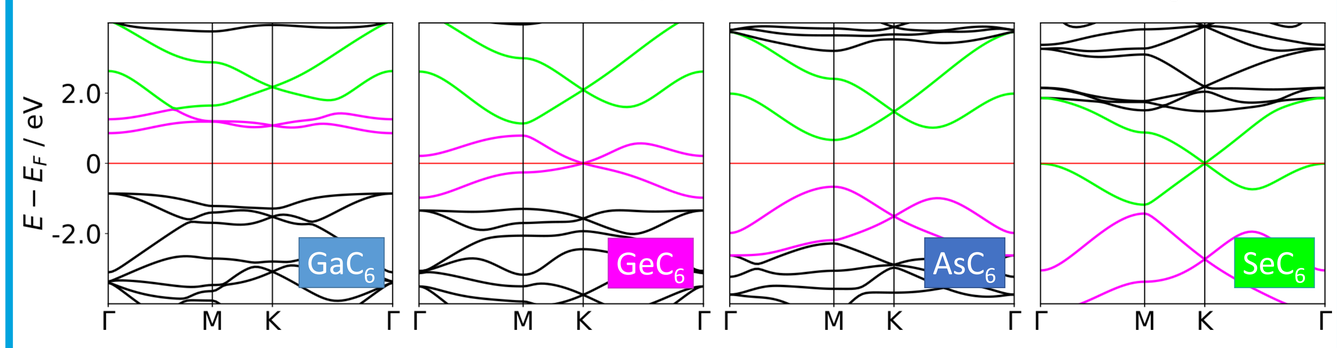
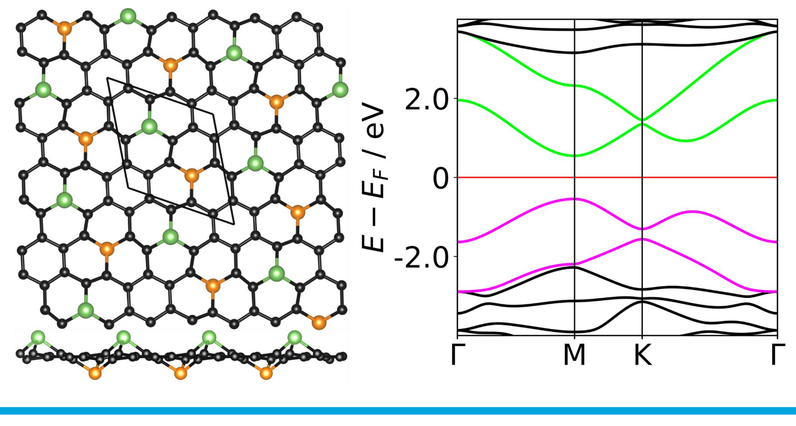


Fig. 2: Band structures for (from left to right): GaC_6, GeC_6, AsC_6, and SeC_6. The energy axes are aligned to fit the axis drawn for GaC_6.

Mixing Heteroatoms

Besides having both heteroatoms per unit cell from one species, they can also be mixed, e.g., as $PAsC_{12}$. Since two group 16 elements are used, it's a direct band gap semiconductor.

Fig. 4: Structure (right, top and side view) and band structure (left) of $PAsC_{12}$. C is black, P is orange, As is green.



Conclusions and Outlook

- PC_6-type materials have two Dirac cones close to the Fermi level.
- Characteristic bands remain the same if the structure remains to be buckled (band structure of flat SiC_6 is slightly different).
- The Dirac cones can be accessed by changing the electron filling with:
  - Substitution strategy: elements from adjacent groups have more or less valence electrons, which affects the position of the Fermi level.
  - Adatom strategy: adsorption of hydrogen to the heteroatoms results in an increase in electron filling.
- Further research: can these strategies be applied to organic topological insulators?

CONTACT PERSON

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