Electronic Structures of Two-Dimensional PC_6-type Materials

Maximilian A. Springer,[1,2] Thomas Brumme,[2] Agnieszka Kuc,[1] Thomas Heine[1,2]
[1]Helmholtz-Zentrum Dresden-Rossendorf, Institue of Resource Ecology,
Permoserstrasse 15, 04318 Leipzig, Germany
[2]TU Dresden, Faculty of Chemistry and Food Chemistry, Bergstrasse 66c, 01069 Dresden, Germany
m.springer@hzdr.de

Electronic properties of π-conjugated 2D materials are dictated by the underlying network topology.[1] Such materials are under investigation for their electron transport properties and potential topological non-triviality. The structure of the recently discovered material family of PC_6[2] corresponds to a $\sqrt{7} \times \sqrt{7}R19.1°$ superstructure of graphene with atoms substituted such that a second honeycomb lattice of phosphorous atoms evolves (distance in xy plane is 3.89 Å, cf. orange network in Fig. 1(a)). The monolayer band structure shows two Dirac points above and below the Fermi level (cf. Fig. 1(b)). PC_6-based structures with the Fermi level at the upper Dirac cone were proposed[3] and potential applications as battery storage material have been described.[4] However, there was no systematic investigation into the fundamental structure-property relationships in the family of PC_6-type materials. Herein, we demonstrate strategies to shift the Fermi level and to tune electronic properties.

References

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Figures

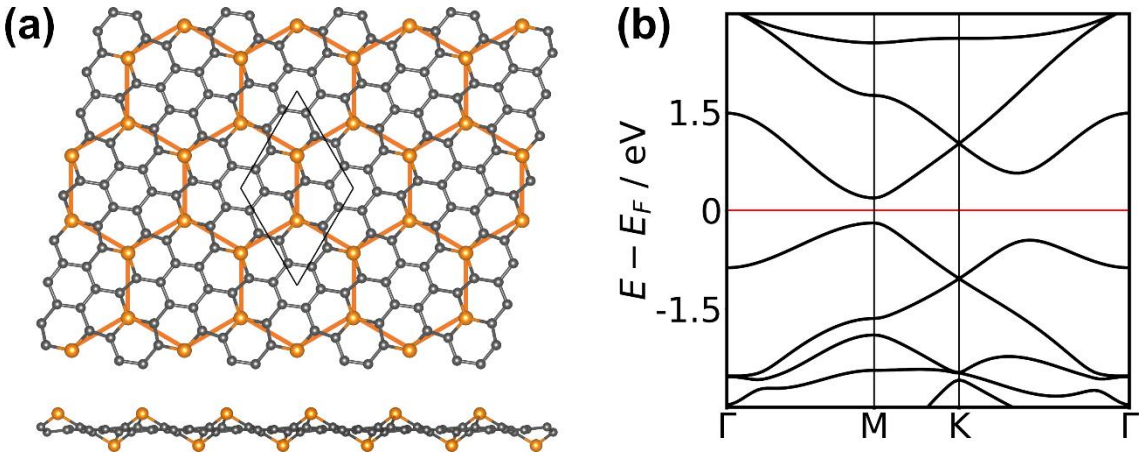

Figure 1: (a) Top and side view of the PC_6 monolayer structure (C: grey, P: orange). It corresponds to a supercell of graphene with atoms substituted to form a second honeycomb lattice (orange lines), (b) band structure of PC_6 monolayer with Dirac cones above and below the Fermi level.