Two-dimensional crystals containing phosphorus

Thomas Heine[1]
Yu Jing,[1] Yandong Ma,[1] Yafei Li[2]

[1] Wilhelm-Ostwald-Institute, Leipzig University, 04103 Leipzig, Germany
[2] Jiangsu Key Laboratory of Biofunctional Materials, Nanjing Normal University, Nanjing, Jiangsu 210023, China

thomas.heine@uni-leipzig.de

Abstract

Phosphorene, a single layer of black phosphorus, has been discovered in 2014 and, despite its low chemical stability, has been considered as promising material for two-dimensional electronics as it has a band gap and high charge carrier mobilities. However, the air-instability of phosphorene strongly limits its application in research, development and potential applications, and thus alterative materials inhibiting similar properties, i.e. high carrier mobility and small band gap, are welcome new members in the family of two-dimensional materials.

We will introduce two new two-dimensional crystals that contain phosphorus. Germanium phosphide, GeP_3 (Figure 1), is a metallic layered material with arsenic-type puckered honeycomb structure that has been experimentally reported in 1970. We show that its single and double layers are low band gap semiconductors, while it becomes metallic for 3 layers and more. Its small band gap, high absorption coefficient and high mobility makes it a promising material for electronic and optoelectronic applications.

We will discuss other isostructural and isoelectronic compounds of the layered materials composed of Group 14/15 elements.

Another interesting layered phosphorus containing material is PdPX, with X=S, Se, Te (Figure 2). Also here, the layered material is known from experiment. The monolayer has electronic properties that appear to be ideal for photocatalytic water splitting with band edges matching the potentials of hydrogen and oxygen evolution reactions. The Pd centres are expected to have beneficial catalytic activity, in particular at the edges of PdPX nanoparticles.

References

[1] Y. Jing, Y. Ma, Y. Li, T. Heine, Nano Lett. 17 (2017), 1833-1838
[2] Y. Jing, Y. Ma, Y. Wang, Y. Li, T. Heine, submitted for publication.

Figures

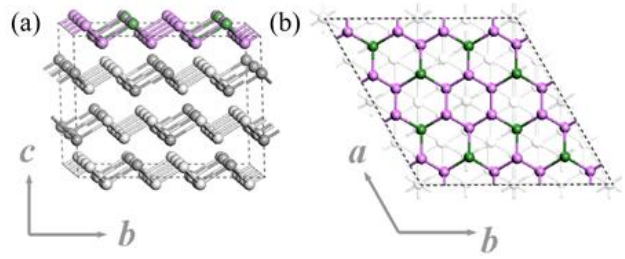

Figure 1. Structure of bulk GeP_3 in a 2×2×1 supercell from side (a) and top (b) views. Pink and green balls represent P and Ge atoms, respectively.

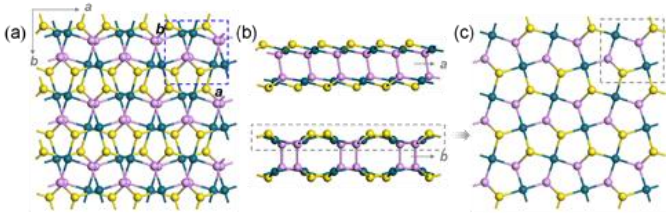

Figure 2. Atomic structure of PdPX ML from top (a) and side (b) views and (c) the sublayer isolated from a ML (unitcell is enclosed by the dashed blue or grey line).