Electronic and optical properties of borophene

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Abstract

Borophene, a two-dimensional monolayer of boron atoms, was recently synthesized experimentally and was shown to exhibit polymorphism [1,2,3]. In its closed-packed triangular form (Fig.1), borophene is expected to exhibit anisotropic metallic character with relatively high electron velocities. At the same time, very low optical conductivities in the infrared-visible light region were predicted. Based on its promising electronic transport properties and its high transparency, borophene could become a genuine lego piece in the 2D materials assembling game known as the van der Waals heterocrystal approach. However, borophene is naturally degraded in ambient conditions and it is therefore important to assess the mechanisms and the effects of oxidation on borophene monolayers (Fig.2). Optical and electronic properties of pristine and oxidized borophene are here [4] investigated by first-principles approaches. The transparent and conductive properties of borophene are elucidated by analyzing the electronic structure and its interplay with light. Optical response of borophene is found to be strongly affected by oxidation, suggesting that optical measurements can serve as an efficient probe for borophene surface contamination.

References

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[2] A.J. Mannix, X.-F. Zhou,B. Kiraly et al., Science, 350 (2015) 1513
[3] B. Feng, J. Zhang, Q. Zhong et al., Nat. Chem., 8 (2016) 563
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Figures

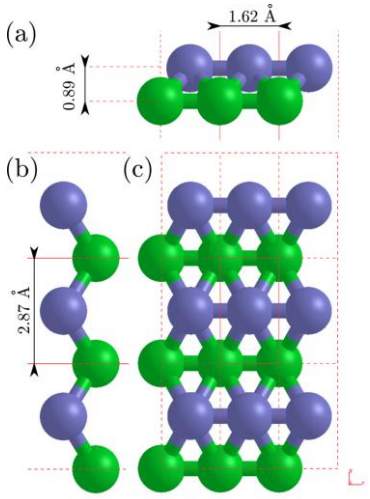

Figure 1: Closed-packed triangular borophene.

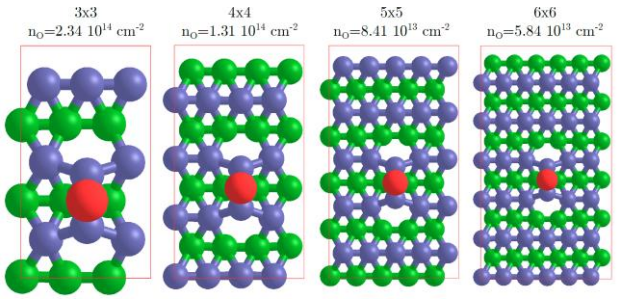

Figure 2: Various densities of oxygen adsorbed onto borophene.