2nd URSI AT-RASC, Gran Canaria, 28 May – 1 June 2018

Electronic and optical properties of phosphorene/graphene van der Waals heterostructures

X. Hu* (1, 2), J. Zheng(2), Z. Sun(1), and Z. Ren(2)
(1) Aalto University, Espoo, Finland, 02150, e-mail: hu.xuerong@aalto.fi; zhipei.sun@aalto.fi
(2) Northwest University, Xi'an, China, 710069, e-mail: zjm@nwu.edu.cn; rzy@nwu.edu.cn

After a series of two-dimensional (2D) layered materials emerging with unique properties [1], van der Waals (vdW) heterostructures have been proposed to design 2D materials with desired properties for various applications [2], such as transistors [3], lasers [4], modulators [5] and detectors [6]. Phosphorene is an increasingly attractive 2D material because of its peculiar properties. Graphene has usually been used to protect phosphorene from degradation for applications [7]. In this work, we systematically investigated the stacking characteristics, electronic structures, band edge alignments and optical properties of all three kinds of stable phosphorene/graphene (P/G) vdW heterostructures in details based on first-principles calculations within the framework of vdW corrected density functional theory [8]. It is interesting that the same stable heterostructures with different lattice mismatch will exhibit different electronic and optical properties. In the heterostructure, the band gap of graphene is almost unchanged when the strain changes from 0 to 3%, while the band gap of phosphorene largely decreases from 1eV to 0.15eV, but always the direct band gap when the strain changes from 0 to 2.8%. In particular, vdW interaction will further increase the gap of phosphorene. We further calculated the optical properties by the photon wavelength dependent dielectric function [9] and find that the strain does not dramatically change the optical properties of graphene but significantly affects that of phosphorene and P/G vdW heterostructures. This work may enhance the understanding of electronic and optical properties of P/G vdW heterostructures and indicate potential reference information for nanoelectronic and optoelectronic applications.

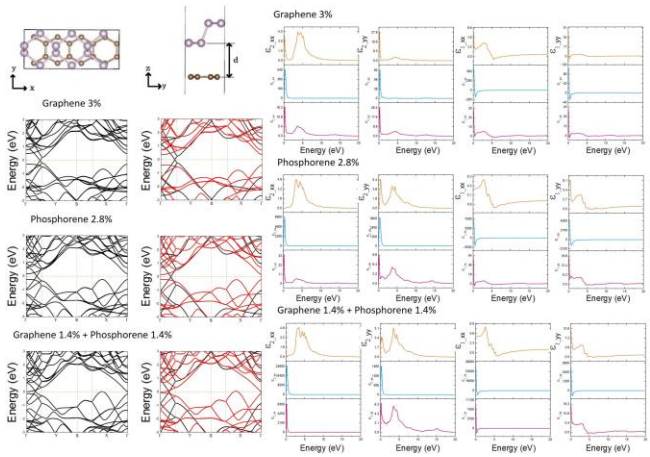

Figure 1. Configuration, band spectrums and corresponding dielectric function (orange line: phosphorene; blue line: graphene; purple line: heterostructure). The percents represent the inhomogeneous strain originating from lattice mismatch.

1. F. Bonaccorso, Z. Sun, T. Hasan, and A. C. Ferrari, "Graphene Photonics and Optoelectronics," *Nature Photonics*, **4**, 31, August 2010, pp. 611-622, doi: 10.1038/NPHOTON.2010.186.

2. A. K. Geim, and I. V. Grigorieva, "Van der Waals Heterostructures," *Nature*, **499**, 25, July 2013, pp. 419-425, doi: 10.1038/nature12385.

3. F. Schwierz, J. Pezoldt, and R. Granzner, "Two-dimensional Materials and their Prospects in Transistor Electronics," *Nanoscale*, **7**, 31, March 2015, pp. 8261-8283, doi: 10.1039/c5nr01052g.

4. H. Chen, J. Yin, J. Yang, X. Zhang, M. Liu, Z. Jiang, J. Wang, Z. Sun, T. Guo, W. Liu, and P. Yan, "Transition-metal dichalcogenides Heterostructure Saturable Absorbers for Ultrafast Photonics," *Optics Letters*, **42**, 1, November 2017, pp. 4279-4282, doi: 10.1364/OL.42.004279.

5. Z. Sun, A. Martinez, and F. Wang, "Optical Modulators with 2D Layered Materials," *Nature Photonics*, **10**, 31, March 2016, pp. 227-238, doi: 10.1038/NPHOTON.2016.15.

6. F. H. L. Koppens, T. Mueller, Ph. Avouris, A. C. Ferrari, M. S. Vitiello, and M. Polini, "Photodetectors based on Graphene, other Two-dimensional Materials and Hybrid Systems," *Nature Nanotechnology*, **9**, 6, October 2014, pp. 780-793, doi: 10.1038/NNANO.2014.215.

7. Y. Cai, G. Zhang, and Y. Zhang, "Electronic Properties of Phosphorene/Graphene and Phosphorene/Hexagonal Boron Nitride Heterostructures," *The Journal of Physical Chemistry C*, **119**, 27, May 2015, pp. 13929−13936, doi: 10.1021/acs.jpcc.5b02634.

8. J. Klimes, D. R. Bowler, and A. Michaelides, "Van der Waals Density Functionals Applied to Solids," *Physical Review B*, **83**, 25, May 2011, pp. 195131 (13), doi: 10.1103/PhysRevB.83.195131.

9. M. Gajdoš, K. Hummer, G. Kresse, J. Furthmüller, and F. Bechstedt, "Linear Optical Properties in the Projector-Augmented Wave Methodology," *Physical Review B*, **73**, 17, January 2006, pp. 045112 (9), doi: 10.1103/PhysRevB.73.045112.