Abstract

Project Code: MRG6180157

Project Title: Design of Electronic Properties of *h*-BN/Blue Phosphorene van Der Waals Heterostructure: First-Principles Study

Investigator: Asst. Prof. Dr. Thanayut Kaewmaraya

E-mail Address: Department of Physics, Faculty of Science, Khon Kaen University, Muang Khon Kaen, Khon Kaen, 40002
thakaew@kku.ac.th

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Abstract:

Recent achievements of fabricating phosphorene, a quasi-single layer of phosphorus with the two-dimensional (2D) planar geometry, have attracted significant interests in devising high-performance (opto) electronics due to its semiconducting feature and ultrafast carrier mobility. Despite such benefits, phosphorene suffers from the rapid degradation in the ambient air to subsequently form insulating phosphorus oxides and eventually lost its profitable characters. On the basis of the *ab-initio* density functional theory (DFT), this research project presents the fundamental electronic and optical properties of the artificial BN-phosphorene van der Waals heterostructures (vdWHs) in which BN is exploited as both the protective layer and the electronic controller. The findings reveal that BN is a proper air-resistant layer because of the intrinsically weak vdW forces between BN and phosphorene sheets that negligibly perturb the host properties. Substitutional doping of carbon into BN can further modulate the electronic and optical properties of vdWHs to be used as promising solar absorbers with the upper bound of 22% theoretical conversion efficiency. Furthermore, the current project reports the potential functionality of phosphorene as chemical gas sensors. This material offers the exceptional selectivity and sensitivity for detecting toxic NO_2 even at the ultralow gas concentration of part-per-billion (ppb), surpassing the detectability of most conventional sensors based on transition oxides. The academic merit of this project is demonstrated by an obligatory international publication in Applied Surface Science (Q1, IF = 5.1) and this work was presented in an international conference. The other by-product publication is currently under review in Journal of Hazardous Materials (Q1, IF = 7.4).

Keywords: Phosphorene, Degradation, Gas sensors