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Electronic and optical properties calculation of blue phosphorus/tetragonal ZnO 2D heterostructure using hybrid density functional theory

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Two dimensional (2D) materials have drawn a lot of attention due to the outstanding properties apart from their bulk counterpart. Since the discovery of the graphene, many 2D materials have been synthesized such as BN, MoS_2, WS_2, and ZnO. These new 2D materials open the opportunity in manufacturing the next generation nano-scale electronic devices. Recently, novel 2D materials, i.e. black phosphorus (black-P) and blue phosphorus (blue-P), were fabricated. The theoretical calculation predicted that blue-P has a wider band gap and higher hole mobility than those of the black-P. The band gap of monolayer blue-P is indirect while that of the black-P is direct. Nevertheless, both blue-P and black-P have poor structural stability under the presence of water and oxygen molecules. To improve their robustness on structural volatility, the blue-P(black-P)/hexagonal ZnO 2D heterostructure was suggested due to the strong chemical stability of the 2D hexagonal ZnO. Moreover, previous calculation showed that this heterostructure gives versatile properties and applications. For instance, it was found that the blue-P interfacing with hexagonal ZnO has indirect band gaps (with a type-II band alignment), but changes to direct band gap when applying external electric field. This then suggest its band gap tunable capability which is useful in the multifunctional device designing. In addition, in our previous work, the tetragonal ZnO monolayer was found to have higher electron mobility than that of the hexagonal ZnO, while their structural stabilities are comparable. Therefore, in this work, the 2D heterostructure of blue-P/tetragonal ZnO was studied and the electronic structures were extracted via hybrid density functional theory to investigate the ZnO structural effects. From the calculation, the results show that the blue-P/tetragonal ZnO 2D heterostructure has direct band gap and its energy gap is lower than that of the blue-P/hexagonal ZnO. The band structure also shows that the blue-P/tetragonal ZnO heterostructure has both high electron- and hole-mobility, which is useful for the charges transportation in photoelectric devices. The high electron-mobility was found to originate from the contribution of ZnO at the conduction band minimum (CBM). On the other hand, the high hole-mobility originates from the contribution of blue-P at the valence band maximum (VBM). Moreover, the blue-P/tetragonal ZnO 2D heterostructure was found to be more stable than that of the parent structures, which shows its potential for implementation in the nano-optoelectronic devices.

Author: SUPATUTKUL, Chumpol

Co-authors: PUNYA JAROENJITTICHAI, Atchara; PRAMCHU, Sittichain; LAOSIRITAWORN, Yongyut

Presenter: SUPATUTKUL, Chumpol

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