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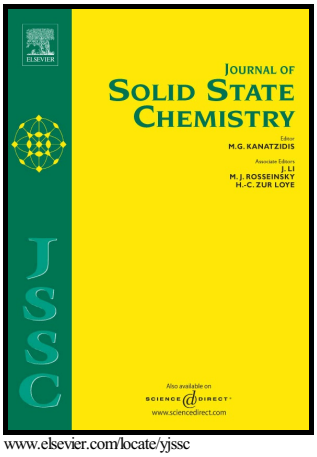

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Electronic properties of blue phosphorene/transition metal dichalcogenides van der Waals heterostructures under in-plane biaxial strains

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Abstract

Using first-principles density functional theory, we have investigated the atomic structural and electronic properties of blue phosphorene/transition metal dichalcogenides BP/XT_2 (X = Mo, W; T = S, Se) van der Waals (vdW) heterostructures under in-plane biaxial strains. Our results demonstrate that the strain can effectively tune the band gap of BP/XT_2 heterostructures and maintain their high carrier mobility. In addition, $BP/MoSe_2$, BP/WS_2 and BP/WSe_2 vdW heterostructures exhibit indirect-to-direct band gap transitions when the compressive strains reach to the critical values. Moreover, the BP/WT_2 (T = S, Se) heterostructures are type-II vdW heterostructures and could be technologically applied as photocatalytic materials. And BP/MoS_2 heterostructure undergoes a semiconduction type transition (type-I to type-II) under the external ε, which has potential application as an on-off switch in the photocatalytic material. These results show rich behavior of the strain-based in blue phosphorene/transition metal dichalcogenides vdW heterostructures.

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