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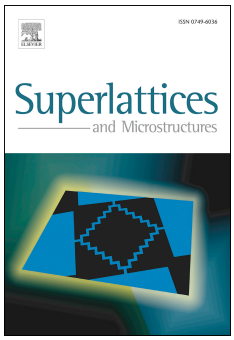

First principles study of the electronic properties and band gap modulation of two-dimensional phosphorene monolayer: Effect of strain engineering

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First principles study of the electronic properties and band gap modulation of two-dimensional phosphorene monolayer: Effect of strain engineering

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Abstract

The effect of strain on the structural and electronic properties of monolayer phosphorene is studied by using first-principle calculations based on the density functional theory. The intra- and inter-bond length and bond angle for monolayer phosphorene is also evaluated. The intra- and inter-bond length and the bond angle for phosphorene show an opposite tendency under different directions of the applied strain. At the equilibrium state, monolayer phosphorene is a semiconductor with a direct band gap at the Γ-point of 0.91 eV. A direct-indirect band gap transition is found in monolayer phosphorene when both the compression and tensile strain are simultaneously applied along both zigzag and armchair directions. Under the applied compression strain, a semiconductor-metal transition for monolayer phosphorene is observed at -13% and -10% along armchair and zigzag direction, respectively.