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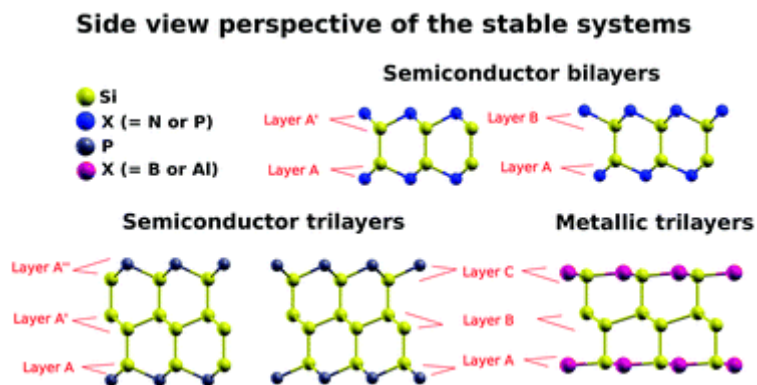
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Functionalized few-layer silicene nanosheets: stability, elastic, structural, and electronic properties

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Abstract

This paper presents an *ab initio* investigation, performed in the framework of density functional theory, on the properties of functionalized few-layer silicene nanosheets, denoted as Si_2X_2 bilayers and Si_4X_2 trilayers with $\text{X} = \text{B}, \text{N}, \text{Al}$, and P . Searching for stable phases, we computed the structural, energetic, thermodynamic, dynamic, elastic, and electronic properties of those systems in several stacking configurations, labeled as AA' , AB , $\text{AA}'\text{A}''$, and ABC . The results revealed that $\text{AA}'\text{-Si}_2\text{N}_2$, $\text{AB-Si}_2\text{N}_2$, $\text{AA}'\text{-Si}_2\text{P}_2$, and $\text{AB-Si}_2\text{P}_2$ bilayers, as well as $\text{ABC-Si}_4\text{B}_2$, $\text{ABC-Si}_4\text{Al}_2$, $\text{AA}'\text{A}''\text{-Si}_4\text{P}_2$, and $\text{ABC-Si}_4\text{P}_2$ trilayers are all dynamically stable, based on their respective phonon dispersion spectra. Particularly, there is scarce literature regarding functionalized trilayer silicene systems and, in this work, we found four new nanosheet systems with interesting physical properties and promising applications. Additionally, according to their standard enthalpies of formation and by exploring their electronic properties, we established that those structures could be experimentally accessed, and we discovered that those silicene nanosheets are indirect band gap semiconductors when functionalized with N or P atoms and metallic with B or Al ones. Finally, we envision potential applications for those nanosheets in alkali-metal ion batteries, van der Waals heterostructures, UV-light devices, and thermoelectric materials.



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