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Tuning the electronic property of two dimensional SiSe monolayer by in-plane strain

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Abstract

Using first-principles calculations, the electronic properties of SiSe monolayer under in-plane strains are studied. It is found that the band gap of SiSe monolayer is increased linearly under the tensile strains along armchair direction. The tensile strain of 7% along zigzag direction makes a transition of band gap from indirect to direct. Under the biaxial compressive strains from 0% to -5%, we found that the band gap of SiSe monolayer is decreased continuously. Moreover, the SiSe monolayer exhibits metallic behavior under the -5% biaxial compressive strain.

Keywords: monolayer SiSe; electronic property; first-principles; in-plane strain

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