Electronic and magnetic properties of silicene monolayer under bi-axial mechanical strain: A first principle study

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The mechanical control of the electronic and magnetic properties of 2D Van-der-Waals heterostructures enables the development of spintronics-related technologies such as memory and quantum-computer devices.

Using the density functional theory, we investigated the structural, electronic and magnetic properties of silicene monolayer with substituted impurity atoms X (X=Fe, Co, and Cr), and under small biaxial strain ($|\epsilon| \leq 8\%$). Our results indicate that the X-doped silicene nanosheets are either magnetic metal or half-metal without strain. We will show that with the tensile strain increasing, the magnetic moment concerning the horizontal dimer substitution has sustained variations and preserves the metallic behaviour. However, it increases slightly through the monomer, and vertical dimer substitution and the system shows a weak semiconductor feature in $\epsilon \geq 8\%$. We will also show that the largest semiconductor band-gap is 0.4 eV at 8% tensile strain for vertical Fe-doped. Finally, biaxial compressive strain leads to emerging fluctuating changes in the magnetic moment, whereas monomer Co-doped disappears in higher strains. Meanwhile, the half-metal behaviour under the compressive strain transforms to a semiconductor for monomer Co and vertical dimer Cr substitution at -4% and -2%, respectively.

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