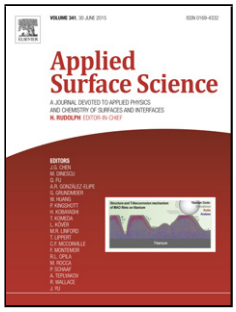

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Tunable electronic and optical behaviors of two-dimensional germanium carbide

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Abstract

The electronic and optical properties of two-dimensional graphene-like germanium carbide (2D-GeC) are calculated using first-principle calculation based on density functional theory. Monolayer GeC has a direct band gap of 2.19 eV. The imaginary part of the dielectric function shows a wide energy range of absorption spectrum for monolayer GeC. Tunable band structures are found for monolayer GeC through in-plane strain. In addition, the band structures and optical properties of bilayer GeC under strain along the c axis are analyzed. Multilayer GeC exhibits a direct band gap like monolayer GeC, and new options of interband transitions are found between layers. The results suggest that 2D-GeC could be a good candidate for optoelectronic such as light-emitting diodes, photodiodes, and solar cells.

Key words: two-dimensional germanium carbide; density-functional theory; electronic properties; optical properties; bilayer GeC.

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