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Band gap tuning of Ge/SiC bilayers under an electric field: a density functional study

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Many studies show that the van der Waals (vdW) bilayers comprised of different types of chemically different two-dimensional (2D) materials display excellent electronic and optical properties, which would be considered as a promising way to construct nanoelectronic and optoelectronic devices. Modulation of the band gap with the help of geometrical strain or an external electric field makes 2D nanosheets particularly interesting materials for nanoscale applications. Therefore, we examine the possible modulation of electronic structure of the Ge/SiC vdW bilayer (shown in Fig. 1a) under the application of electric field (E-field) by using first-principles methods. Without an E-field, the system shows a band gap of 126 meV at the equilibrium state, as shown in Fig. 1b. While an E-field is applied, the band gap of Ge/SiC bilayer exhibits an interesting phenomenon, as shown in Fig. 1c. The trend of band gap is approximately symmetric at 0.0 V/Å. While the E-field is in the range 0.0 to −0.40 V/Å, the band gap increases slightly and reaches a maximum of about ~378 meV at −0.20 V/Å. Conversely, the band gap decreases monotonously with increasing E-field strength, ranging from 378 to 0 meV for −0.20 to −0.40 V/Å, and the Ge/SiC bilayer further becomes a zero-gap structure at −0.40 V/Å. A similar phenomenon appears, while E-field changes from 0.0 to +0.40 V/Å. The band gap reaches a maximum of about ~315 meV at +0.10 V/Å, then the band gap decreases to zero at +0.40 V/Å. From our current calculations, it is clearly that the E-field could regulate the band gap of Ge/SiC vdW heterostructures effectively. With an E-field, the band gap first increases and then decreases, which shows a parabola-like relation with the E-field. Moreover, the band structures and PDOS calculations indicated that different states of Ge, Si, and C atoms contributed to such significant variations of band gap. Our finding is very important for the potential applications of Ge/SiC vdW heterostructures in future nanoelectronic devices.

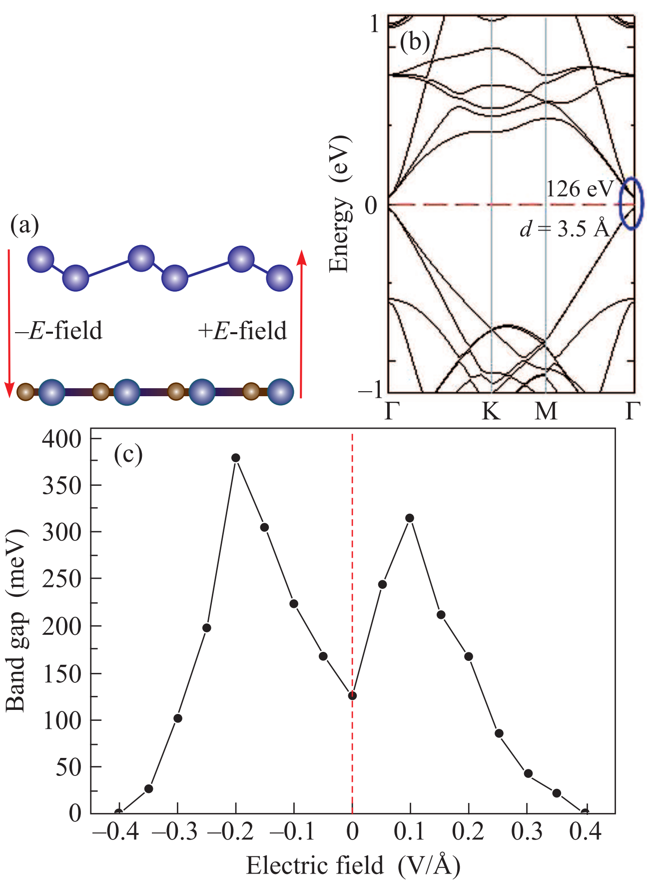

Fig. 1. (Color online) (a) – Side view of the Ge/SiC vdW heterostructures, and the electric field (E-field) along the c-axis. (b) – Band structure of the vdW heterostructures at the equilibrium state. (c) – Band gap of the nanocomposite as a function of the E-field

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