Supporting Information

for

Computational exploration of two-dimensional silicon diarsenide and germanium arsenide for photovoltaic applications

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Additional computational data

We studied the variation of the band gap as a function of the tensile strain by using the PBE functional (Figure S1). It can be seen that the band gap variation depends on the viewing direction along the lattice. External strain on semiconductor nanostructures influences electronic properties and, thereby, optical properties [1,2].

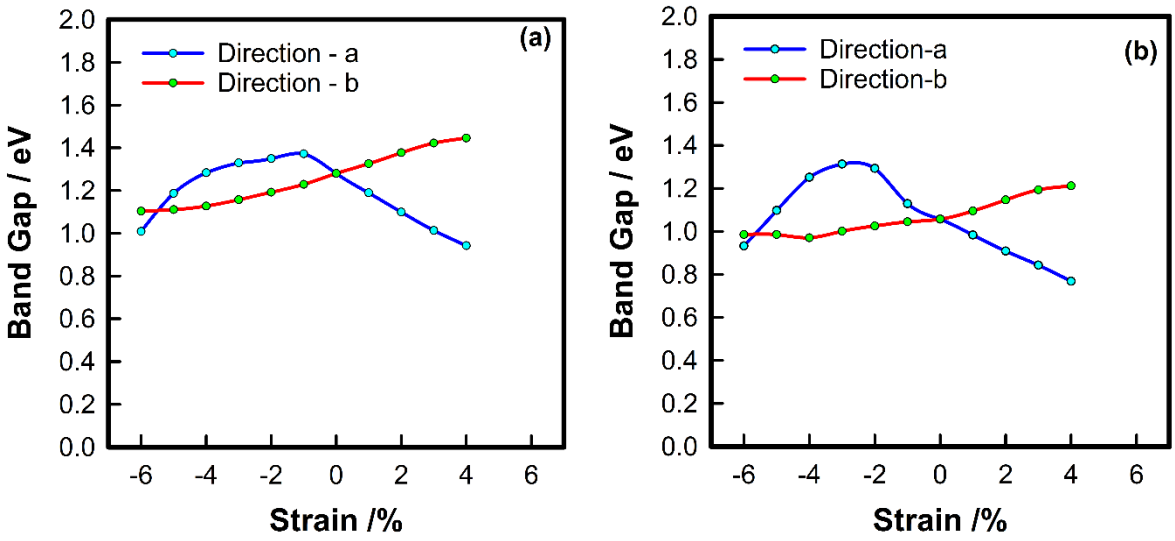

Figure S1: Band gap as a function of biaxial strain calculated with the PBE functional for monolayers of (a) $SiAs_2$ and (b) $GeAs_2$.

References

1. Zhou, M.; Duan, W.; Chen, Y.; Du, A., *Nanoscale* **2015,** *7*, 15168-15174. doi:10.1039/C5NR04431F

2. Ma, F.; Zhou, M.; Jiao, Y.; Gao, G.; Gu, Y.; Bilic, A.; Chen, Z.; Du, A., *Sci. Rep.* **2015,** *5,* 17558. doi:10.1038/srep17558