

Supporting Information

Theoretical Insights into Z-Scheme BAs/GeC van der Waals Heterostructure for High-Efficiency Solar Cell.

Khawla Chaoui ^{a,*}, Kamel Zanat ^a, Warda Elaggoune ^b, Luc Henrard ^c, Mohamed Achehboune ^c.

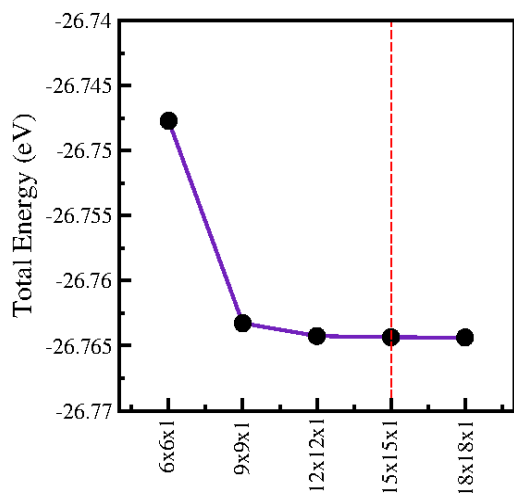
^a Guelma Physics Laboratory (GPL), Département des sciences de la matière, Faculté des mathématiques, de l'informatique et des sciences de la matière, Université 8 Mai 1945, BP 401, Guelma, Algeria.

^b Laboratoire de Physique des Matériaux (L2PM), Faculté des mathématiques, de l'informatique et des sciences de la matière, Université 8 Mai 1945, BP 401, Guelma, Algeria.

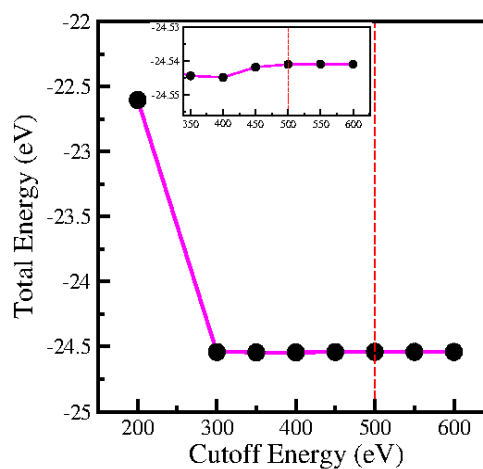
^c Department of Physic, Namur Institute of Structured Matter, University of Namur, Rue de Bruxelles 61, 5000, Namur, Belgium.

*Electronic mail : chaoui.khawla@univ-guelma.dz

Keywords: First-principles calculations; 2D heterostructures; Z-scheme band alignment; Biaxial strain; Photovoltaic applications.



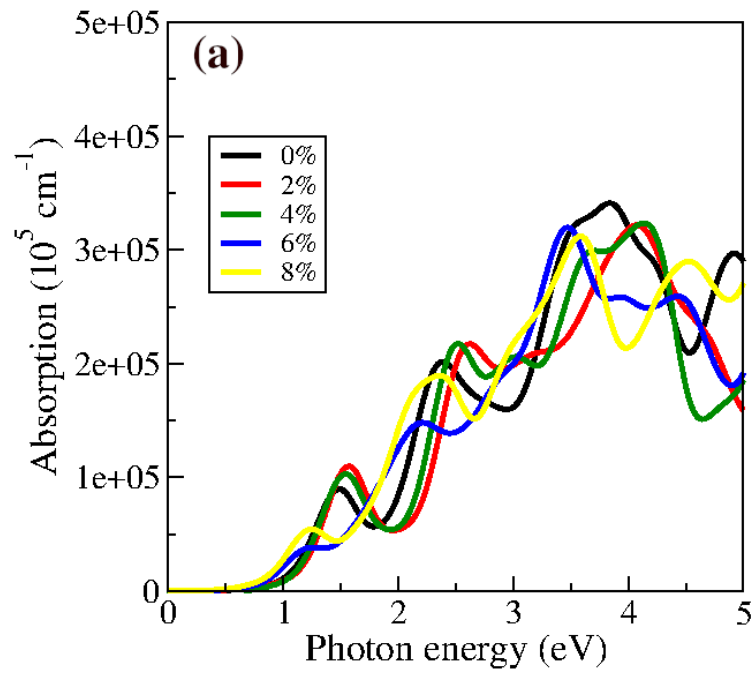
(a)



(b)

S1 The variation of total energy as a function of (a) Kpoints (b) cutoff using HSE06 functional.

S2 Optical properties under biaxial tensile strain



The variation of the absorption of BA/GeC heterostructure under biaxial tensile strain.