First-Principles Study of Doped GaAs Nanowires

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We study theoretically the problem of doping of GaAs nanowires in which one cation/anion is substituted by a dopant atom. We consider several elements, which are usually used to obtain p- or n-type conductivity in GaAs, i.e., Si, Be and Sn. We study also the distribution of Au and O atoms. Si as a IV group element can act both as a donor (by substituting the group III cation) and as an acceptor (by substituting the group V anion). With the calculations we want to answer the question:

Has the crystal structure of nanowire an impact on the segregation and formation energies of various impurities in GaAs nanowires?

Segregation energy – which site in the wire the dopant prefers to substitute:

$$E_S = E_i - E_{center} \quad i = 1,\ldots,15,\ldots,20$$

Formation energy – the energy needed to substitute cation/anion by a dopant in the wire:

Neutral impurity: $\Omega(X^0_{cat/an}) = E_{doped} - E_{undoped} + \mu_{cat/an} - \mu_{Si}$

Charged impurity: $\Omega(Si^-_{an}) = \Omega(Si^0_{an}) + E_F(Si^0_{an}) - \mu_e$ $\quad \Omega(Si^+_{cat}) = \Omega(Si^0_{cat}) - E_F(Si^0_{cat}) + \mu_e$

E_F – Fermi energy of NW with neutral donor/acceptor

μ_e – electron chemical potential which satisfies the requirement of charge neutrality; $0 \le \mu_e \le E_g$

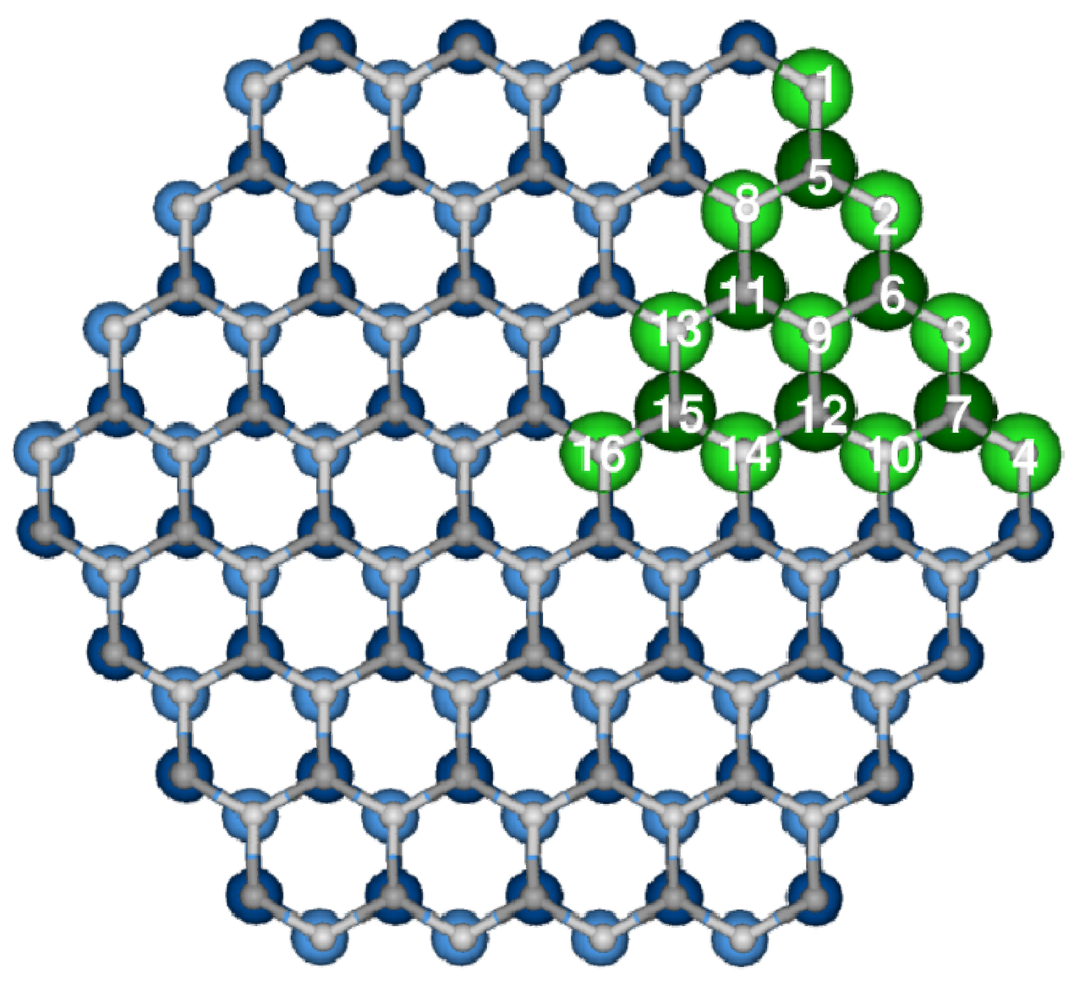
μ_i – chemical potential of *i* atoms (*i = Ga, As*)

μ_{si} – chemical potential of dopant

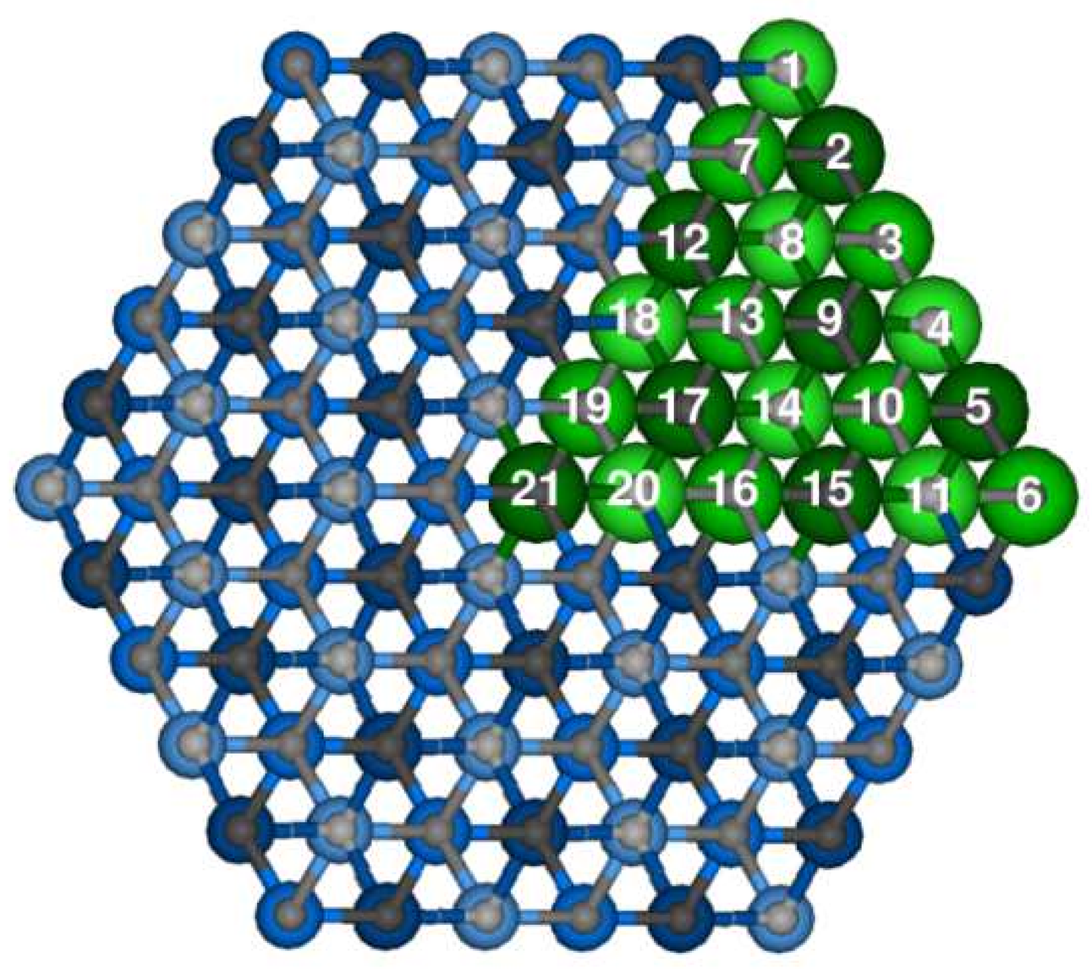
equilibrium condition: $\mu_{cat} + \mu_{an} = \mu_{GaAs}$

$d\mu = (\mu_{cat} - \mu_{an}) - (\mu_{cat(bulk)} - \mu_{an(bulk)})$; **physically accessible region** of $d\mu$: $-\Delta H \le d\mu \le \Delta H$, where

$\Delta H = \mu_{cat(bulk)} + \mu_{an(bulk)} - \mu_{GaAs(bulk)}$ is the heat of formation of GaAs

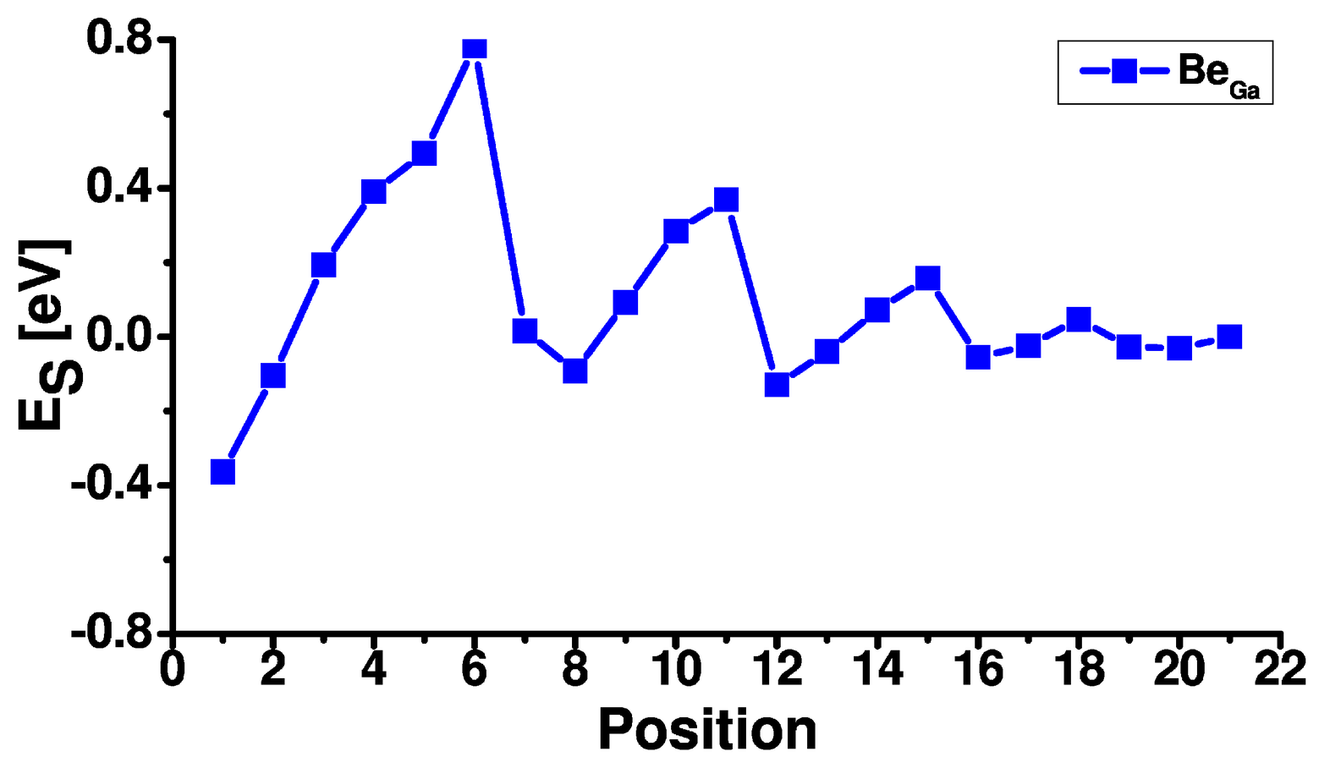


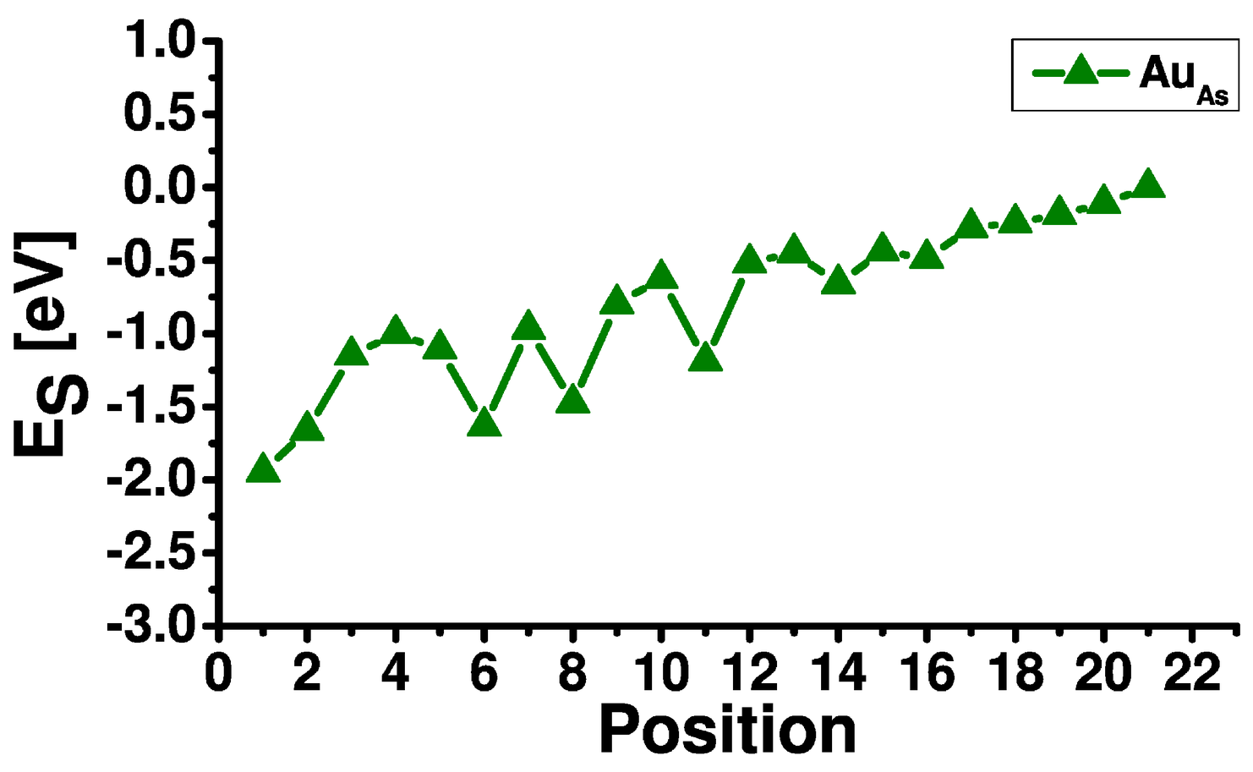
WZ NW

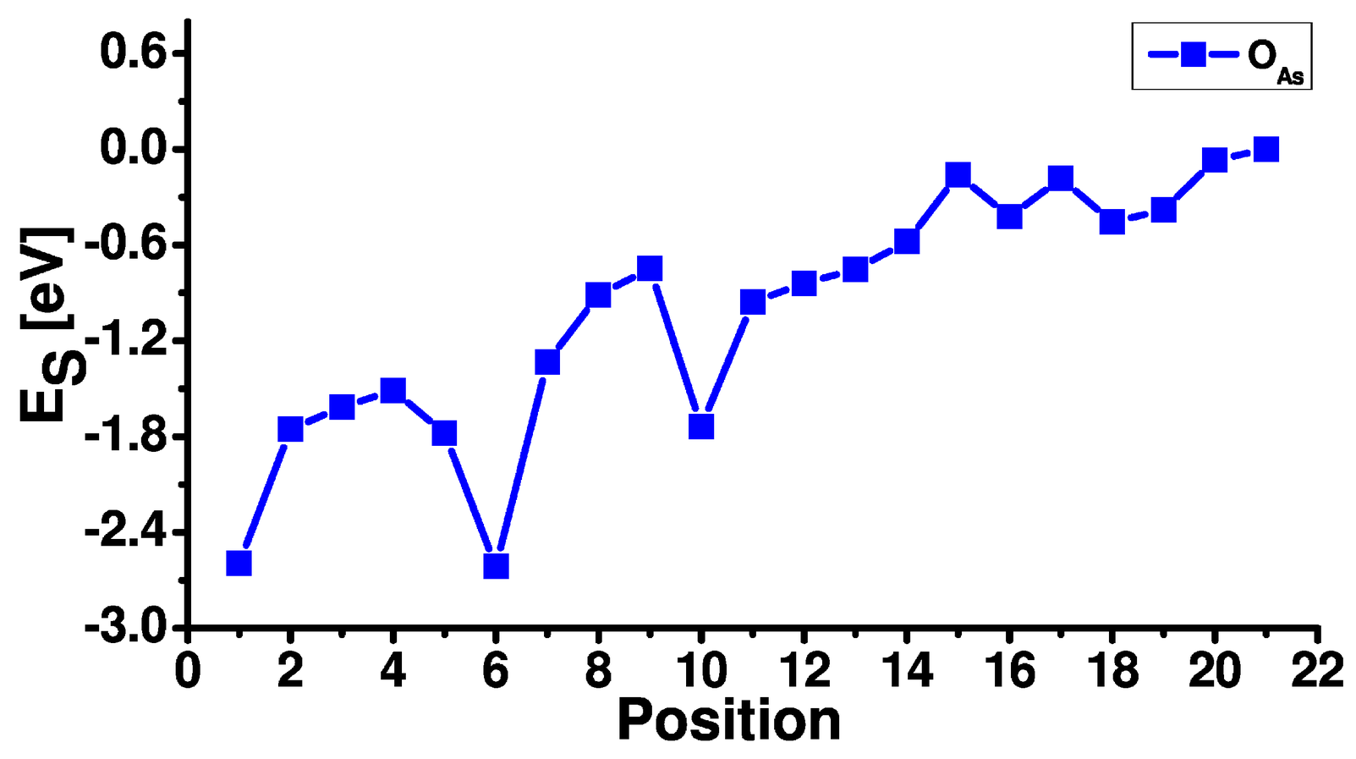


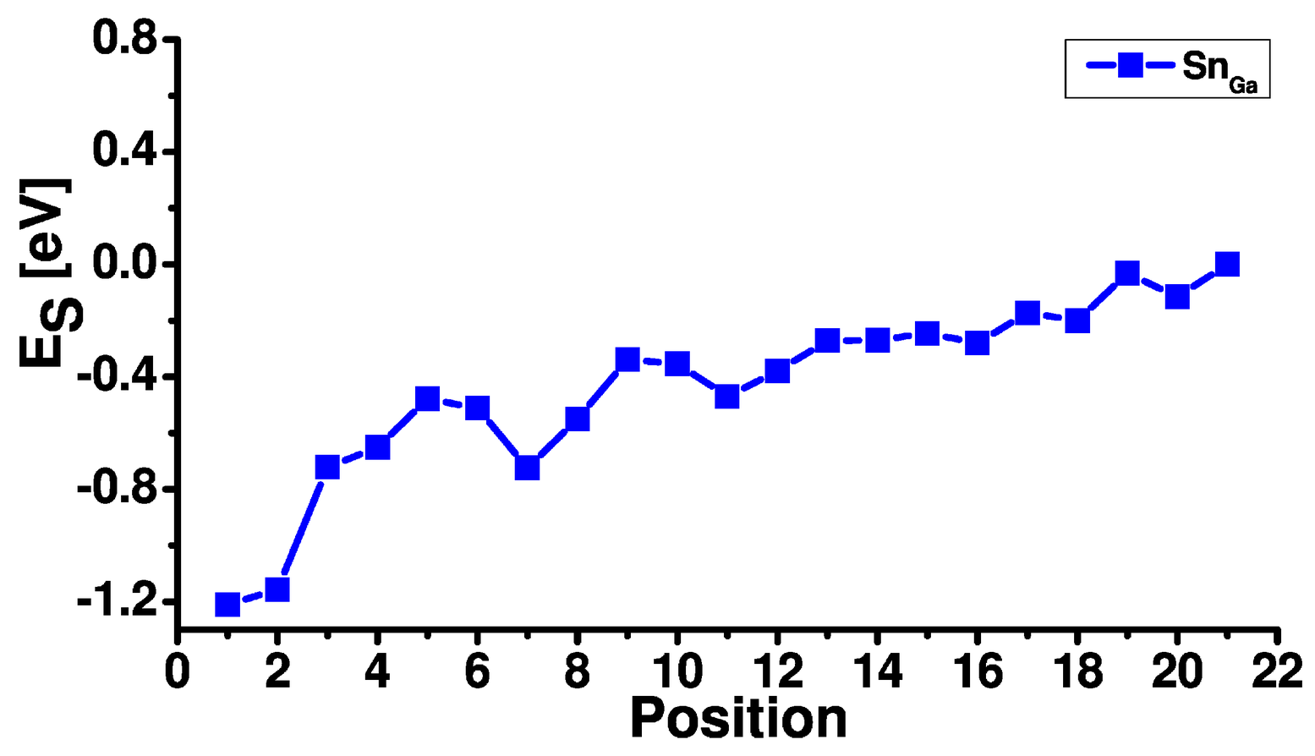
ZB NW

ZB



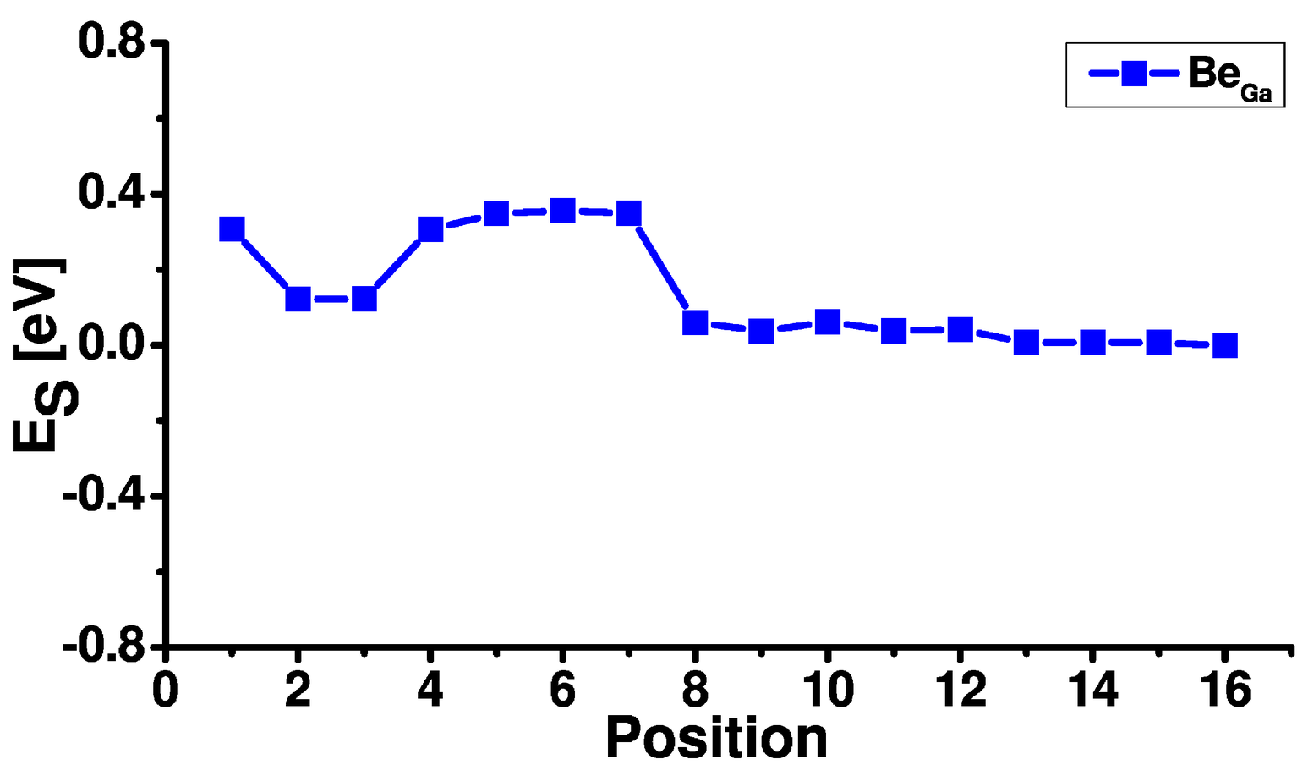


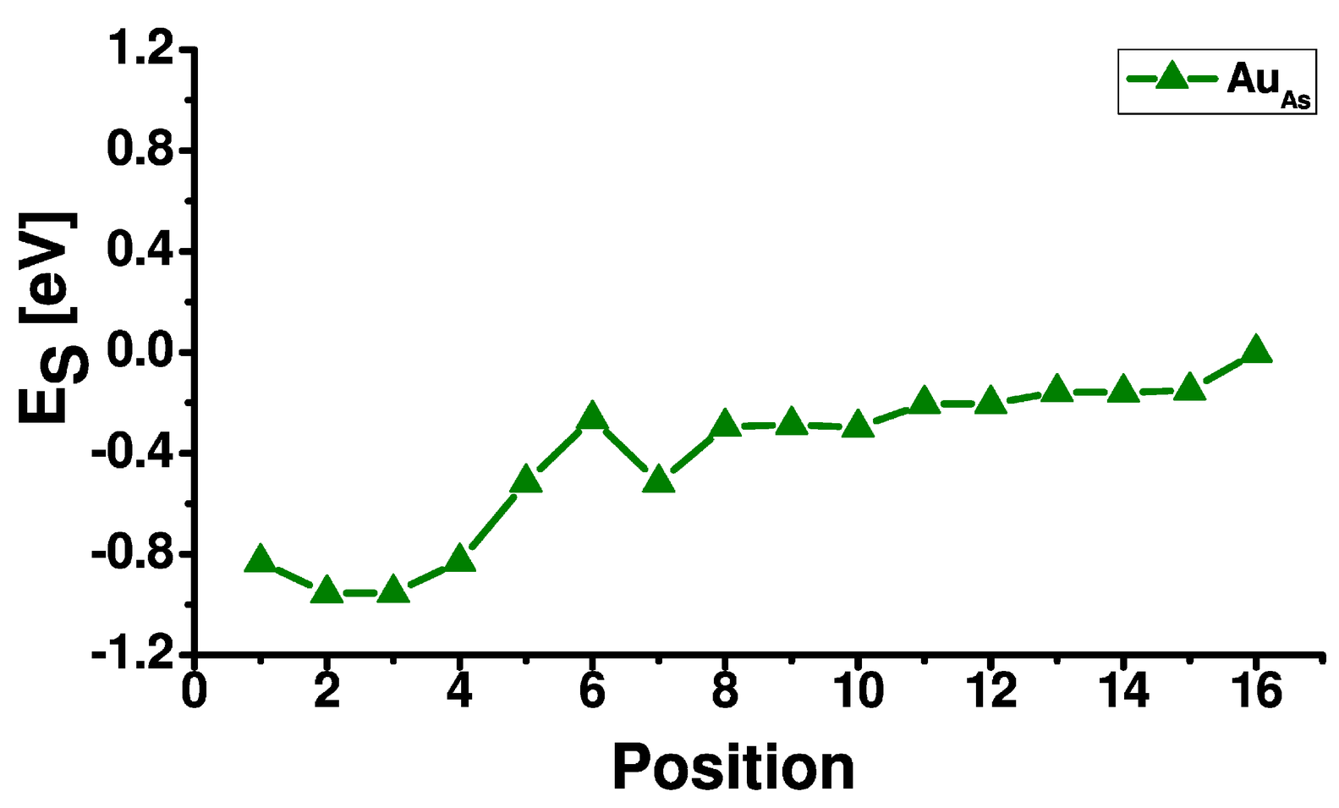


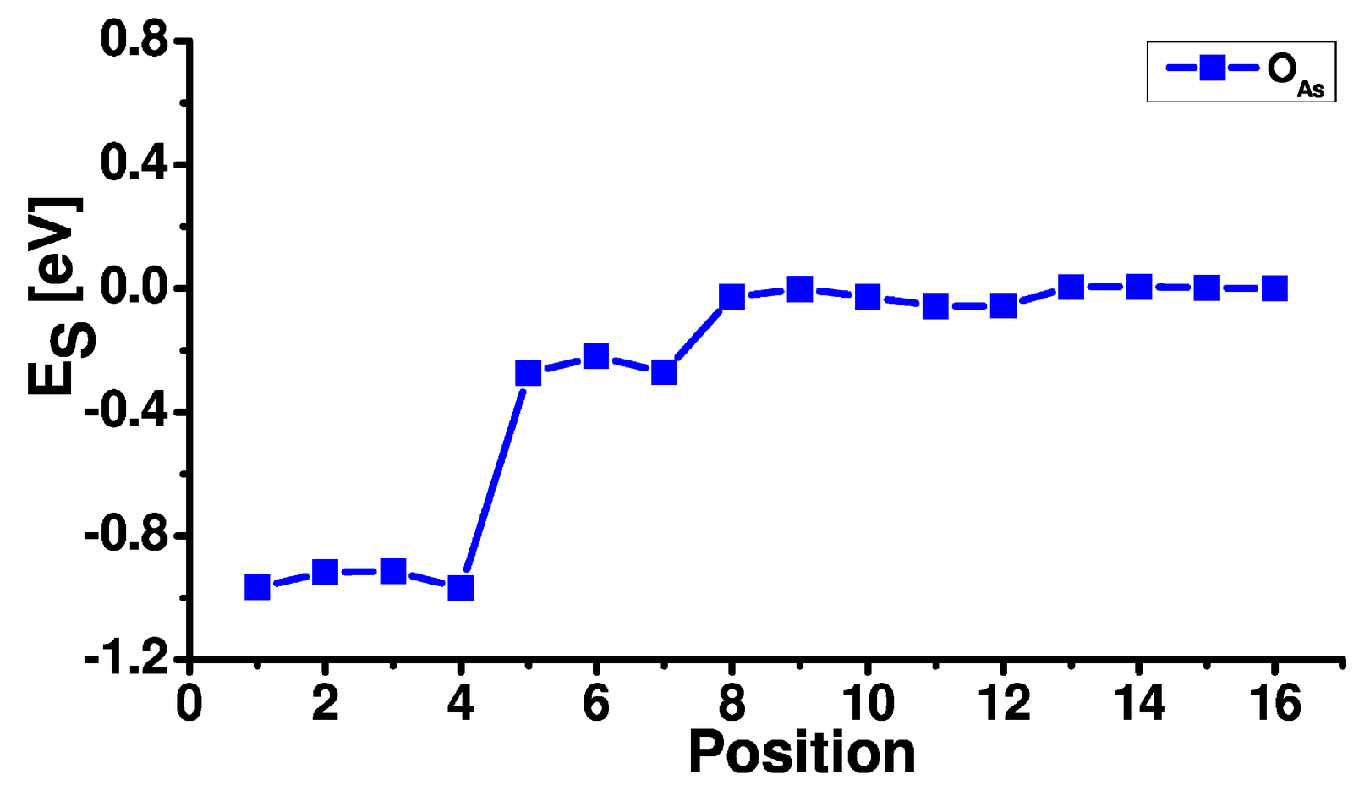


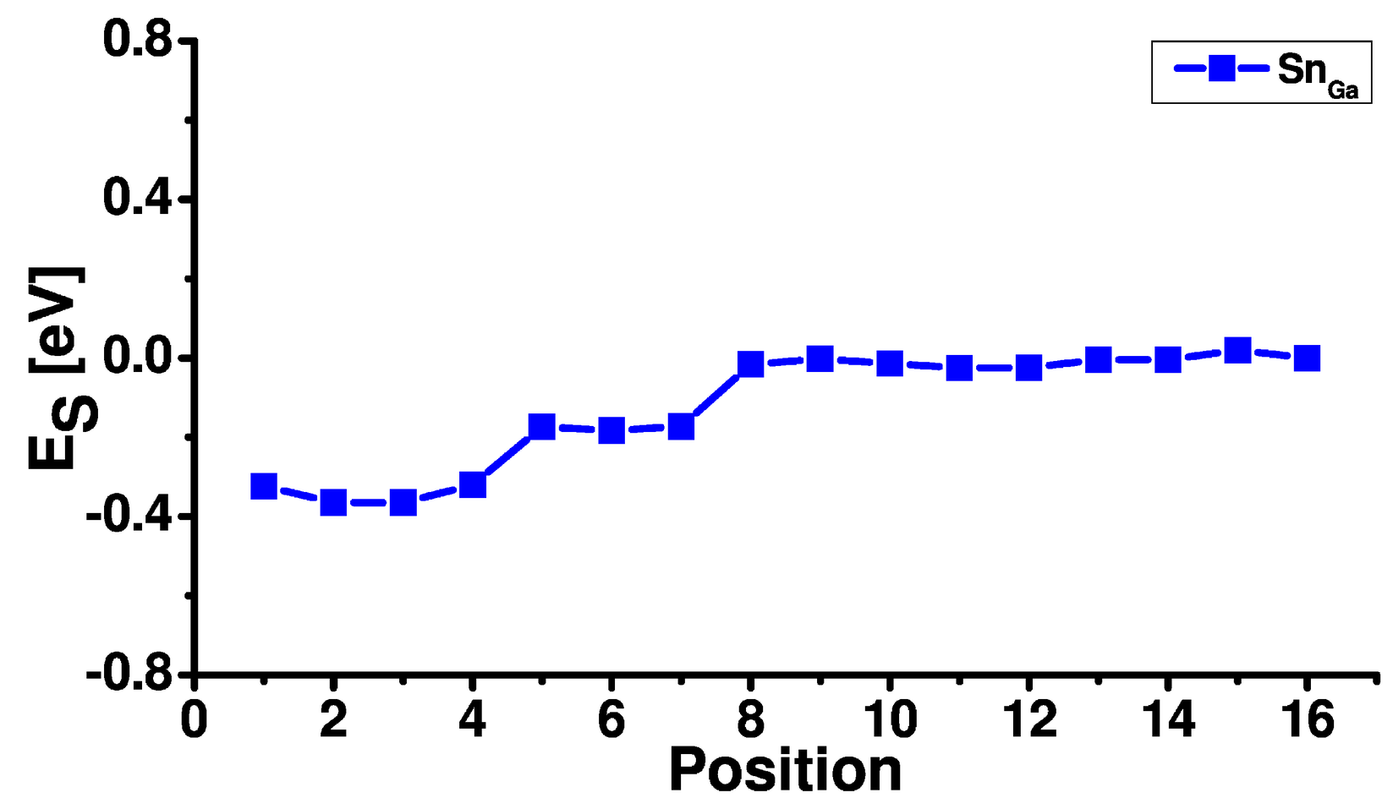
Be **Au** **O** **Sn**

WZ

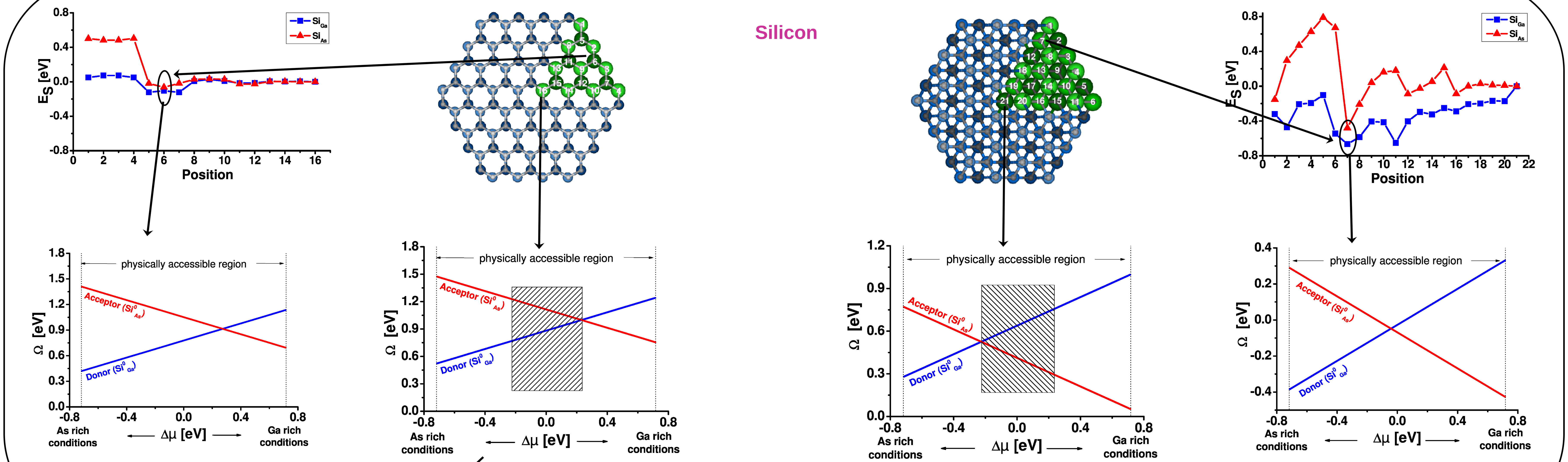




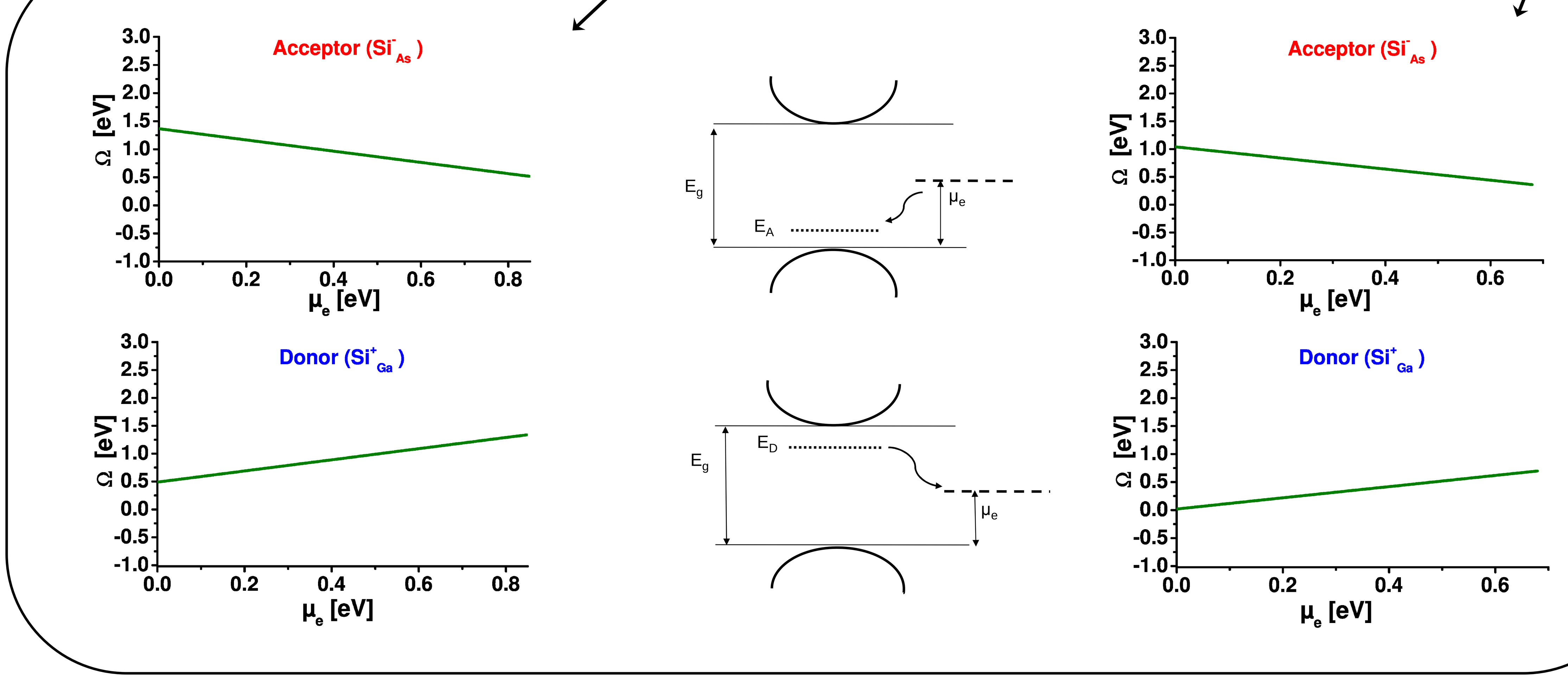




Silicon



For Si near the atom with extra dangling bond Ω<0!



Summary

Crystal structure has an impact on the distribution of impurities and formation energy of doped GaAs NWs !

- While distribution of dopants in WZ NWs is usually more homogenous, the formation energies for most of the impurities are higher in WZ NWs than in ZB NWs
- Si-doping can lead to a p-n junction at the WZ/ZB stacking faults