Supplementary material

November 15, 2022

Internal angles

In Figure S1, we have presented the internal angles for the SiC monolayers considered in this work, also in the table S1 all values for the angles are given. We could see that the interaction between Si and Li atoms leads to densification of the SiC monolayer and that this causes the angles to decrease.

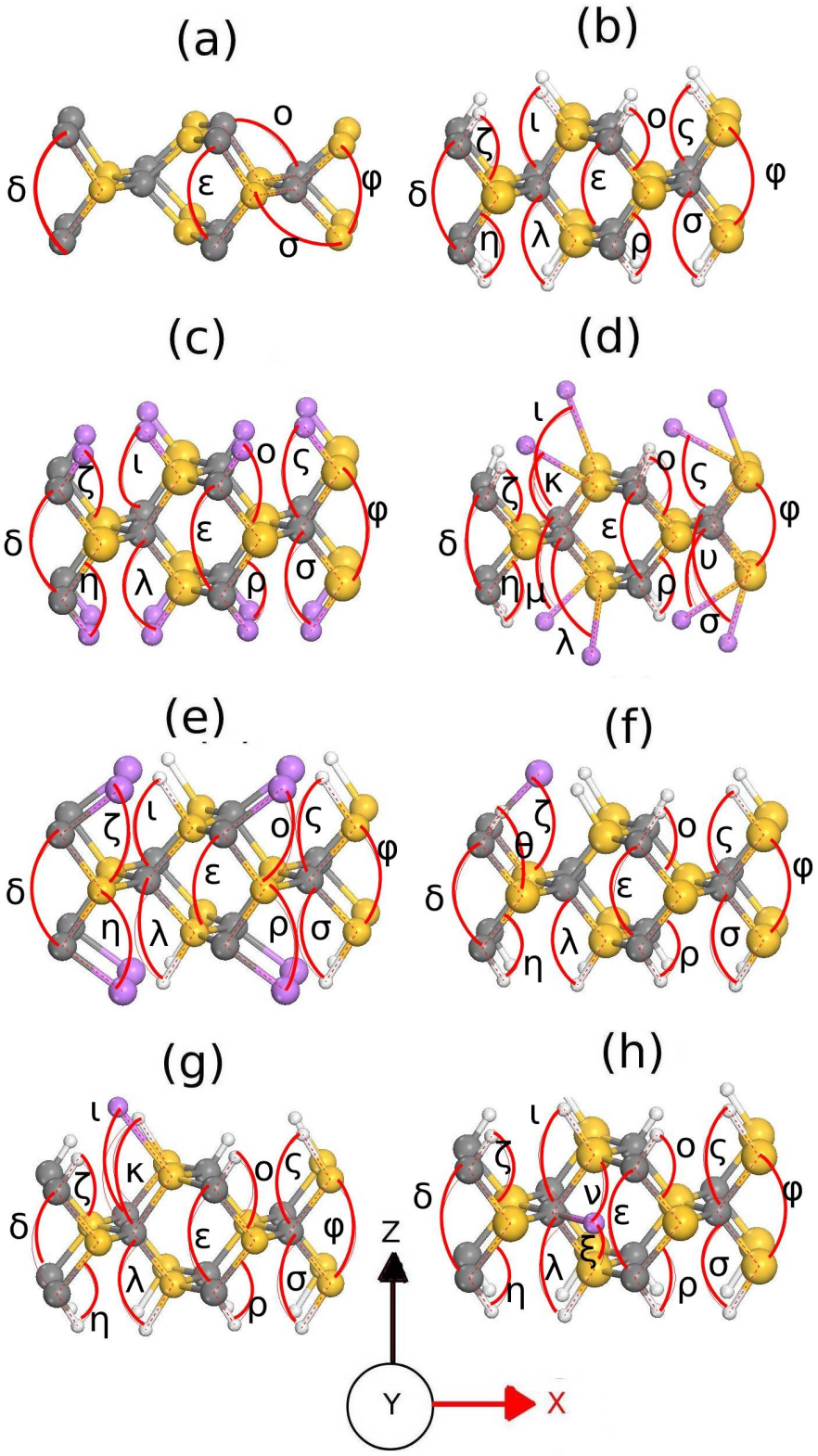

Figure S1: Schematic representation of 3C-SiC (1 1 0) with surfaces different passivations schemes after relaxation (a)Pristine, (b)Full-H, (c)Full-Li, (d)CH+SiLi, (e)CLi+SiH, (f)H+1LiC (g)H+1LiSi, (h)H+Li$_c$. The grey, yellow, white and purple spheres represent the C, Si,H and Li atoms, respectively.

Passivation Scheme	Angles (°)
Pristine	δ=109.47 ϵ= 109.47 o = 109.14 σ= 113.74 φ= 89.72
Full-H	δ=108.9 ζ=108.95 η=109.04 ι=110.53 λ=110.58 ϵ=108.23 o = 108.9 ρ=109.04 ς 110.53 σ=110.58 φ=109.71
Full-Li	δ=108.5 ζ=109.26 η=109.26 ι=109.54 λ=109.54 ϵ=108.5 o = 109.26 ρ=109.26 ς 109.54 σ=109.54 φ=108.9
CH+SiLi	δ=100.373 ζ=112.93 η=109.64 ι=124.48 κ=86.69 μ=92.62 λ=119.46 ϵ=100 o = 113.28 ρ=107.14 ς= 110.53 ν= 118.6 σ=83.46 φ=105.23
	δ=109.17

CLi+SiH	ζ=91.91 η=91.94 ι=105.92 λ=105.89 ϵ=109.17 o = 91.91 ρ=91.94 ς=105.92 σ=105.89 φ=96.78
H+1LiC	δ=104.2 ζ=100.0 θ=109.0 η=109.5 λ=109.8 ϵ=103.3 o =108.3 ρ=108.4 ς=107.4 σ=110.2 φ=104.5
H+1LiSi	δ=102.5 ζ=108.2 η=108.8 ι=109.4 κ=109.4 λ=111.4 ϵ=104.0 o =109.5 ρ=109.7 ς111.6 σ=109.7 φ=104.8
H+Li$_c$	δ=106.1 ζ= 109.4 η=109.4 ι=111.5 λ=111.6 υ=71.9 ξ=71.89 ϵ=101.0 o =107.1 ρ=107.0 ς=110.6 σ=110.6

	φ=105.8

Table S1: Bond lengths between atoms involved in close interaction Si-C, Si-H, Si-Li, C-H,C-Li and the experimental values.

Convergence test

As we could see from the figure S2, the final energy of the system has values from -283.50 eV to -283.34 eV for values below 300 eV. However, if we consider an energy limit higher than 300 eV, there is no significant variation in the final energy. To ensure convergence results without increasing the time required for the calculations, we choose an energy cutoff of 350 eV.

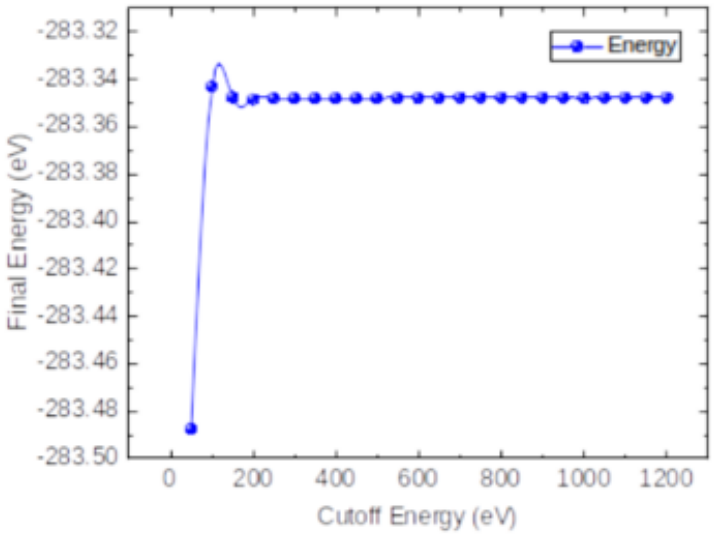

Figure S2: Variation of the final energy in dependency of the cutoff energy for 3C-SiC.

In Figure S3, we have shown the convergence test for different values of k points. The final energy depends on the choice of k points for values below 6 k points mesh, but there is no significant change for values above 6 k points.

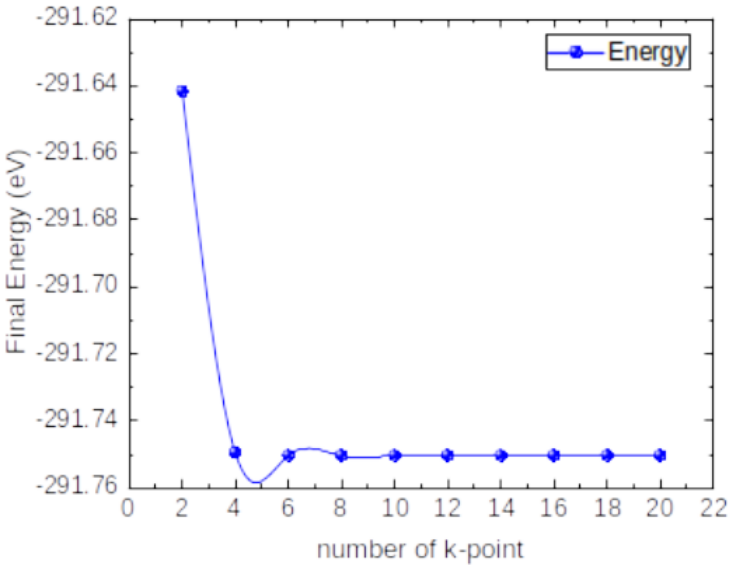

Figure S3: Variation of the final energy in dependency of the k-point mesh for 3C-SiC.