

# Adsorption of alkali and alkaline-earth atoms on Silicon Carbide Monolayer

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Graphene-like materials have attracted considerable attention from fundamental investigations to potential applications due to their intriguing structural, electronic, transport, optics and other quantum effect properties. Silicon Carbide Monolayer (SiC-M) is a material which is convenient for high temperature and high-power device applications, because of its wide band gap [1,2]. The adsorption characteristics of alkali and alkaline-earth ad-atoms on SiC-M (Figure 1) are analysed by means of first-principles calculations. In addition to structural properties, we calculate electronic, and magnetic properties. The investigation of the interaction of SiC-M with metal atoms has a significant importance because of its fundamental relevance to applications in hydrogen storage, catalysis, batteries, and chemical sensors.

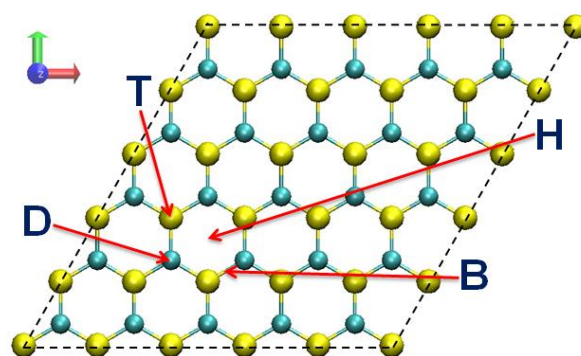
## References

- [1] H. Sahin and F. M. Peeters, *Physical Review B*, **87** (2013) 085423.
- [2] H. Sahin, et al, *Physical Review B*, **80** (2009) 155453.

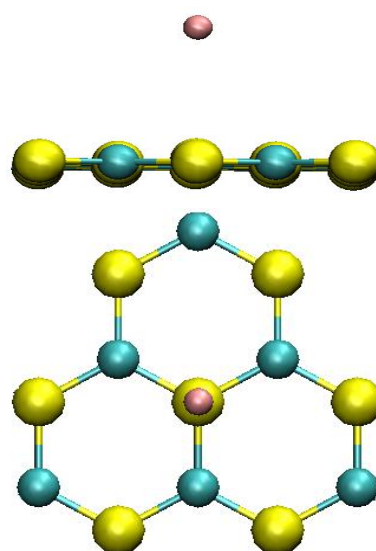
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**Table 1:** Calculated values for adatom adsorption on (5x5) SiC-M; in the best relaxation site top (T), adatom height (h) and adsorption energy of adatom ( $E_{\text{Ads}}$ ).

Adatom	Site	h(Å)	$E_{\text{Ads}}$ (eV)
Li	T	2.43	0.89
Na	T	2.76	0.52
K	T	3.15	0.72
Be	T	2.18	0.49
Mg	T	3.18	0.18
Ca	T	3.01	0.26



**Figure 1:** Atomic structure of a SiC-M (5x5 supercell). The four sites of adsorption: down (D), top (T), hollow (H) and bridge (B) are shown.



**Figure 2:** Side and top view for characteristic adsorption geometries for alkali and alkaline-earth. Cyan, yellow and pink balls represent C, Si and Alkali (Alkaline-earth) atoms, respectively.