Electronic Supplementary Material (ESI) for New Journal of Chemistry.

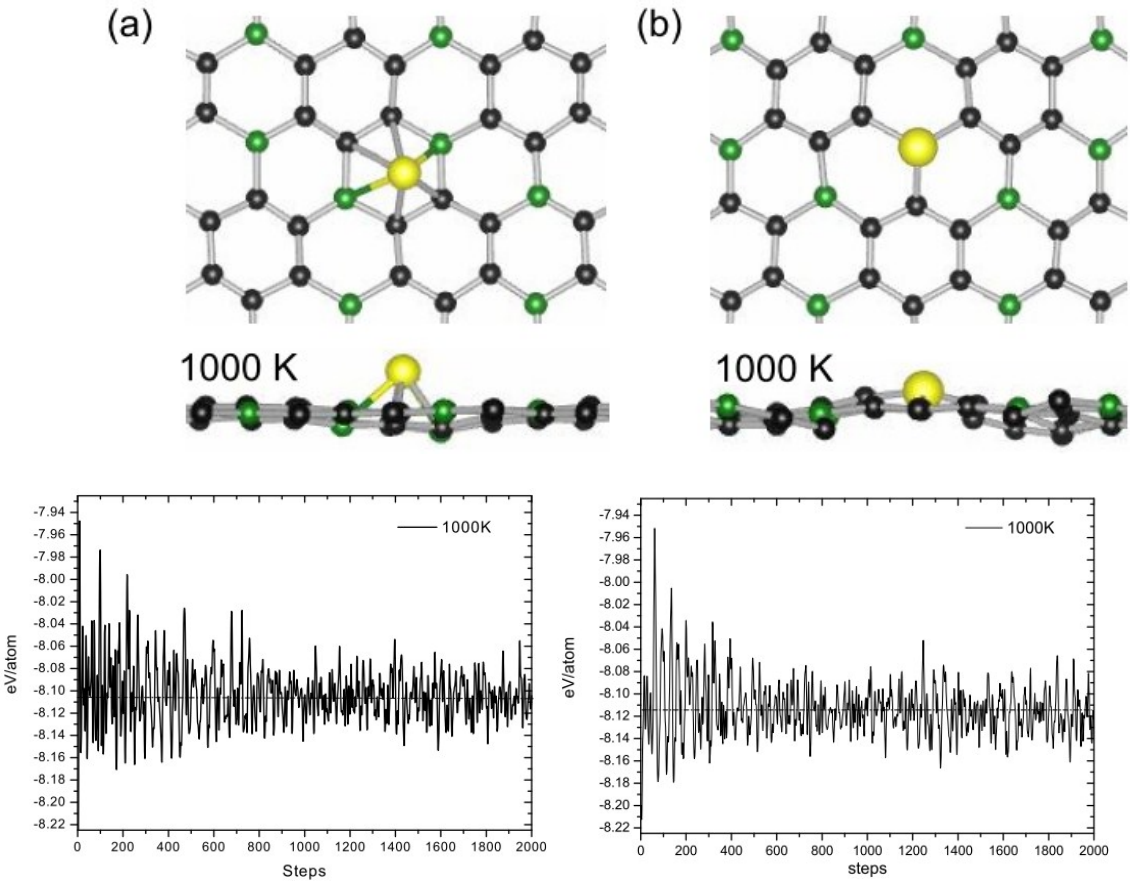

Figure S1 Top and side views of the most stable configurations for (a) Si/pri-BC_3 and (b) Si-BC_3 from the first-principles molecular dynamics simulations at 1000K, respectively. Black, green and yellow balls represent C, B and Si atoms, respectively.

Table S1 The adsorption energy (E_{ads}, in eV), bond length (d_3, in Å) and adsorption height (d_4, in Å) between adsorbed O_2 (or CO) and substrates NM-BC_3 sheet are calculated by GGA-PBE and DFT-D2 methods.

Substrates	Adsorbates	GGA-PBE			DFT-D2		
		E_{ads}	d_3	d_4	E_{ads}	d_3	d_4
Si-BC_3	O_2	1.47	1.45	1.78	1.53	1.45	1.77
	CO	0.41	1.15	1.91	0.46	1.15	1.91
P-BC_3	O_2	0.60	1.56	1.68	0.75	1.56	1.67
N-BC_3	O_2	0.03	1.23	3.24	0.11	1.23	3.23