Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

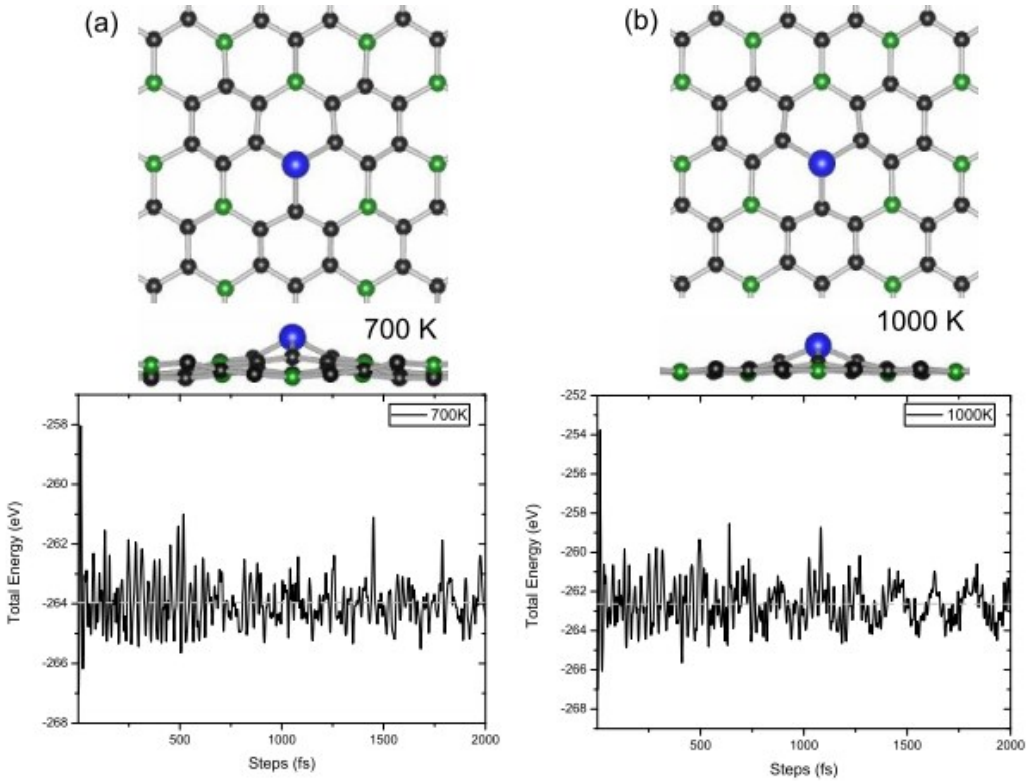

Figure S1 Top and side views of the final Fe-BC_3 structure from the molecular dynamics simulation at (a) 700 K and (b) 1000 K. Black, green and blue balls represent C, B and Fe atoms, respectively.

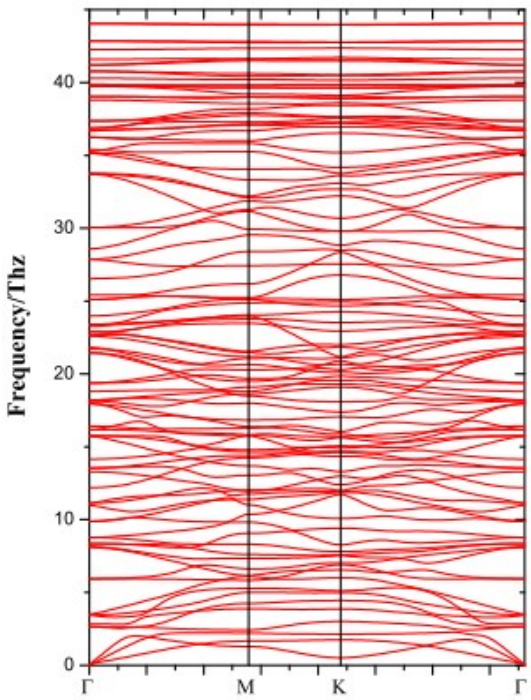

Figure S2 Phonon spectrum of Fe-BC_3 monolayer.

Table S1 The adsorption energy (E_{ads}, in eV) and magnetic moment (M, in u_B) for single Fe atom or gas molecule (CO and O_2) on the BC_3 or Fe-BC_3 nanosheet by using different density functional (GGA-RP and GGA-PBE).

systems	Fe/pri-BC_3		Fe-BC_3		O_2/Fe-BC_3		CO/Fe-BC_3	
	E_{ads}	M	E_{ads}	M	E_{ads}	M	E_{ads}	M
GGA-PBE	2.86	2.0	6.92	1.0	1.20	3.0	0.74	1.0
GGA-RP	2.45	2.0	6.56	1.0	1.34	3.0	0.71	1.0