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

Supplementary information// Point defects in two-dimensional BeO monolayer First-principles study on electronic and magnetic properties

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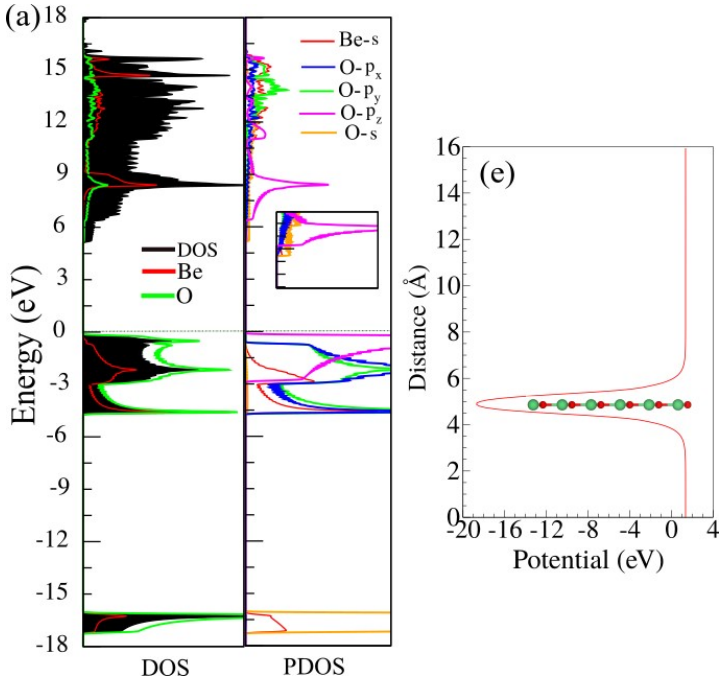

Fig S1. (a) DOS and PDOS and (b) average electrostatic potential of the BeO monolayer

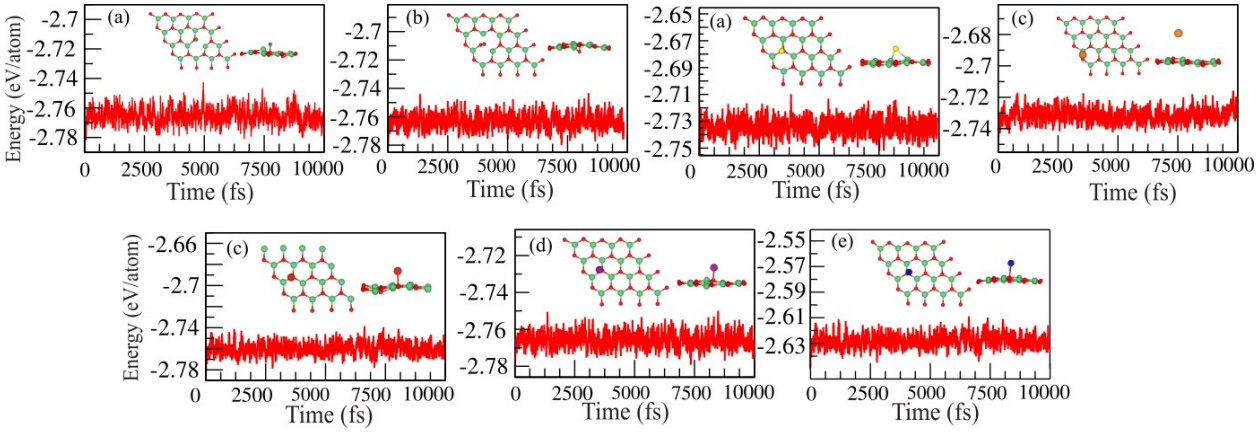

Fig S2. Ab initio molecular dynamics (AIMD) for BeO monolayer adsorbed with (a) B , (b) C , (c) S , (d) Mg , (e) V , (f) Mn and (f) Co adatoms at 400 K temperature. Top and side views of the structure after 5 ps of simulation demonstrated as insets. :

	Bridge	Hollow	Top-Be	Top-O
H	-226.79986	-226.80171	-226.81356	-226.79584
B	-227.26505	-227.27188	-227.26712	-227.25019
C	-228.57306	-227.34615	-227.35984	-228.57189
Si	-227.43793	-226.87725	-226.80313	-227.44542
N	-228.86506	-228.87709	-228.86957	-228.85732
P	-227.64093	-227.66655	-227.65529	-227.66121
F	-227.91526	-227.13484	-227.82862	-227.72799
Cl	-226.70295	-226.40567	-226.41012	-226.70535
O	-229.41337	-228.13366	-228.19826	-229.41191
S	-227.69754	-226.99702	-226.99481	-226.68792
Li	-226.32698	-226.39173	-226.17169	-226.35329
Na	-226.07887	-226.08967	-226.03544	-226.08304
K	-226.01105	-226.01638	-225.98928	-225.99977
Be	-225.97098	-225.80779	-225.79666	-225.99319
Mg	-225.78610	-225.78665	-225.76619	-225.77971
Ca	-225.94999	-225.87383	-225.82106	-225.93941
Al	-226.44405	-226.42363	-225.78822	-226.64154
Sc	-227.70641	-227.99864	-227.94127	-228.32075
Ti	-227.68110	-228.69347	-228.51916	228.64347
V	-229.91424	-229.58288	-229.51520	-229.90358
Cr	-231.34742	-231.35831	-231.31285	-231.13381
Mn	-230.94163	-230.97700	-230.93986	-231.00963
Fe	-229.57614	-229.25488	-229.30856	-229.40020
Co	-228.15407	-228.01995	-227.89633	-228.15256
Ni	-227.31013	-227.30619	-226.68853	-227.30691
Cu	-226.35145	-226.25015	-226.21660	-225.96193
Zn	-225.82199	-225.83848	-225.81957	-225.81967

TableS1: Total energy of various adatoms at four adsorption sites (including Bridge, Hoollow, Top-Be and Top-O) on the BeO monolayer. The most stable site energy indicated by red colour

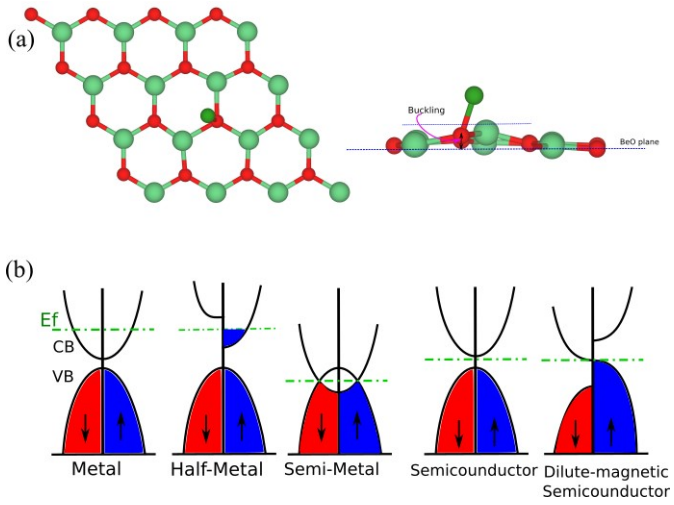

Fig S3. (a) Optimized atomic structure of BeO monolayer with adsorbed B atom at top of O host atom. Buckling of O bonded to B inidicated as shematically. (b) Schematic diagram of different electronic states including of metal, half-metal(HM), semiconductor (SC) and dilute magnetic semiconductor (DMSC).

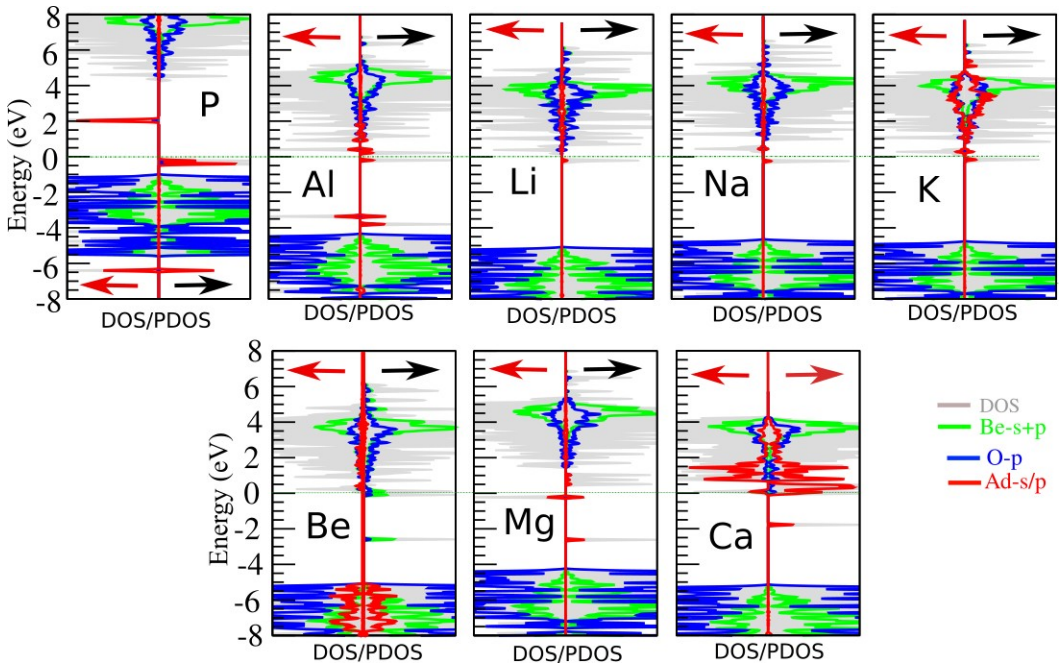

Fig S4. Total DOS and PDOS of different adatom adsorbed on the BeO monolayer

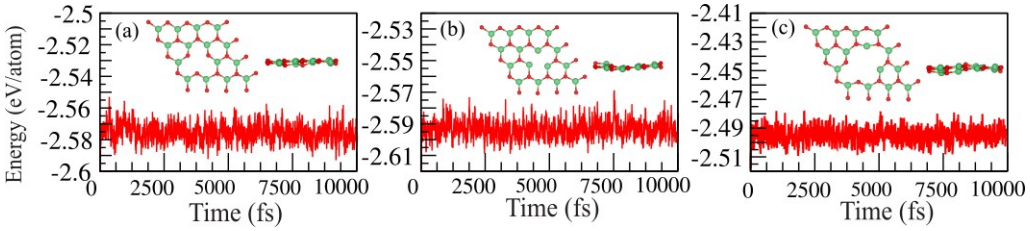

Fig S4. Ab initio molecular dynamics (AIMD) for Be monolayer with (a) a single Be vacancy,

(b) a single O vacancy and (c) double vacancy Be+O defects. at 400 K temperature. Top and side views of the structure after 5 ps of simulation demonstrated as insets.

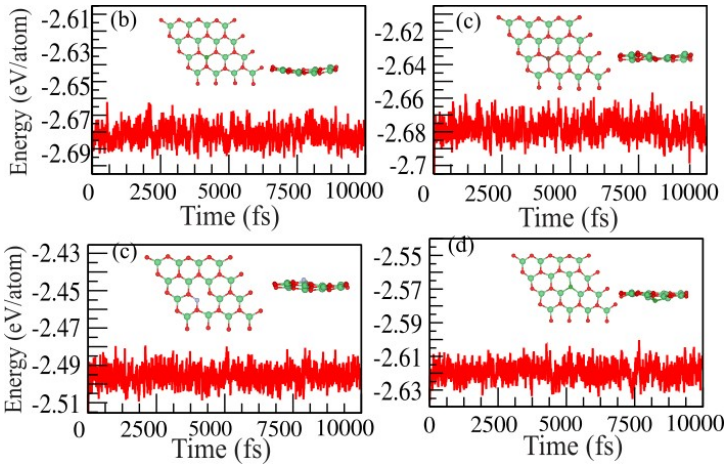

Fig S5. Ab initio molecular dynamics (AIMD) for BeO monolayer doped with
(a) B Be , (b) N Be , (c) C Be , and (d) B O at 400 K temperature. Top and side views of the structure after 5 ps of simulation demonstrated as insets.