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# Robust electronic properties of monolayer BeO against molecules adsorption

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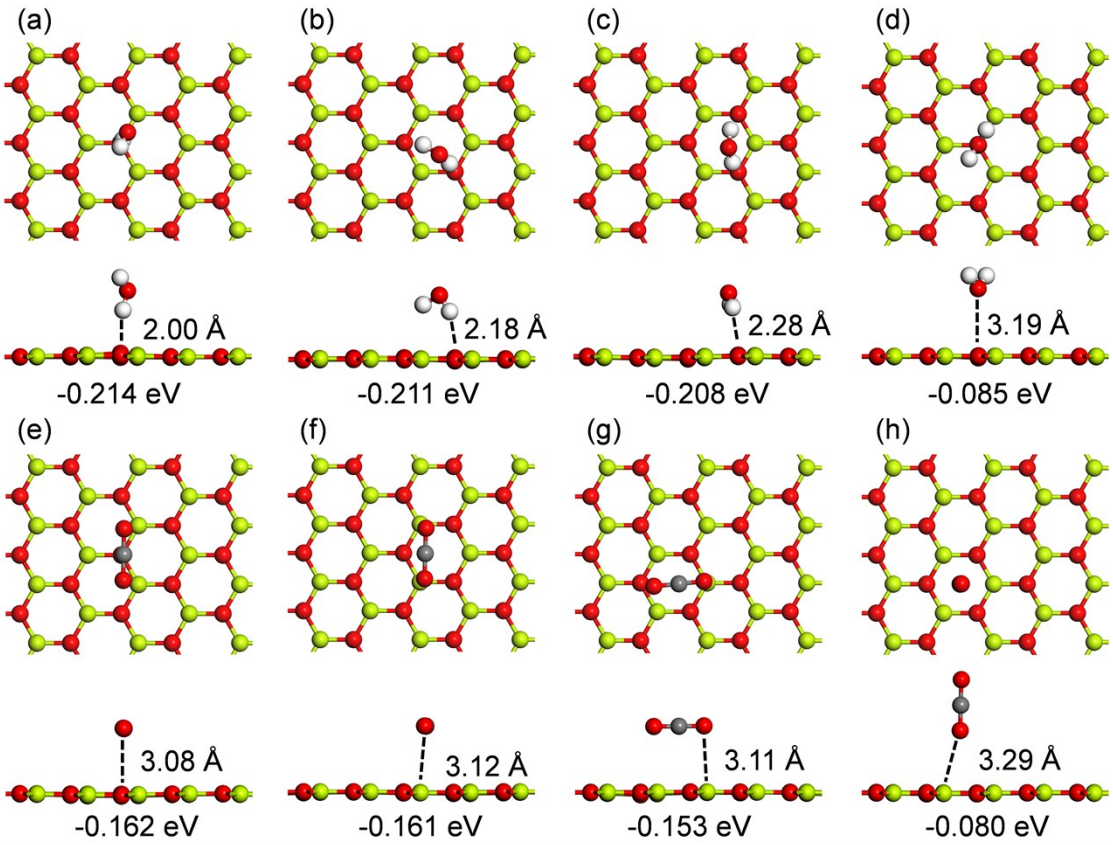


**Figure S1.** Top and side views of other possible structures for gas molecules on pristine BeO monolayer. (a) – (d): $H_2O$ on BeO monolayer. (e) – (h): $CO_2$ on BeO monolayer. The red, green, white and gray balls represent O, Be, H and C atoms, respectively. The shortest distance between the molecule and BeO layer is given indicated by dashed lines. The adsorption energy was given below each structure.

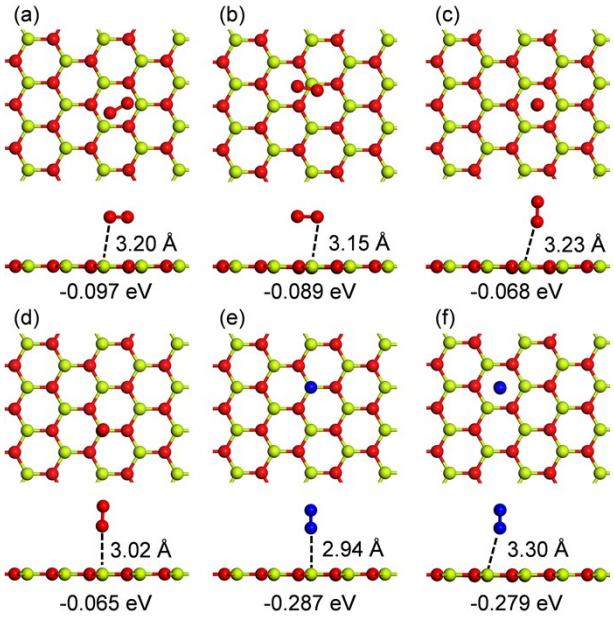


**Figure S2.** Top and side views of other possible structures for gas molecules on pristine BeO monolayer. (a) – (d): $O_2$ on BeO monolayer. (e) – (f): $N_2$ on BeO monolayer. The red, green and blue balls represent O, Be and N atoms, respectively. The shortest distance between the molecule and BeO layer is given indicated by dashed lines. The adsorption energy was given below each structure.

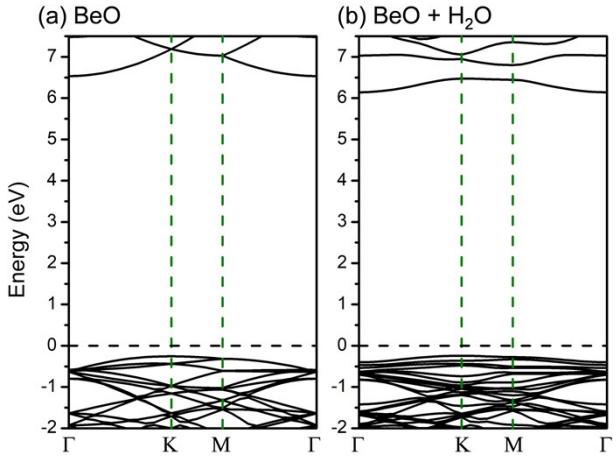


**Figure S3.** Electronic energy band structures calculated with HSE06 functional: (a) pristine BeO monolayer (b) BeO monolayer with the adsorption of a $H_2O$ molecule.

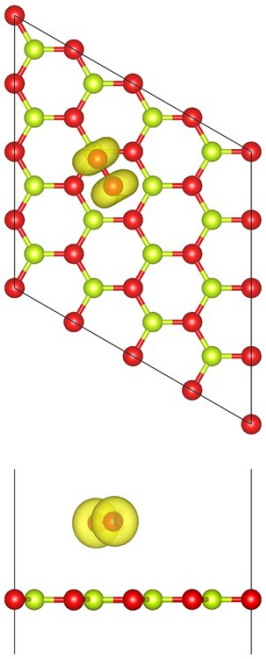

**Figure S4.** Spin charge density of the BeO monolayer with the adsorption of $O_2$. The red and green balls represent O and Be atoms, respectively. The isosurface level is 0.008 |e|/bohr$^3$.

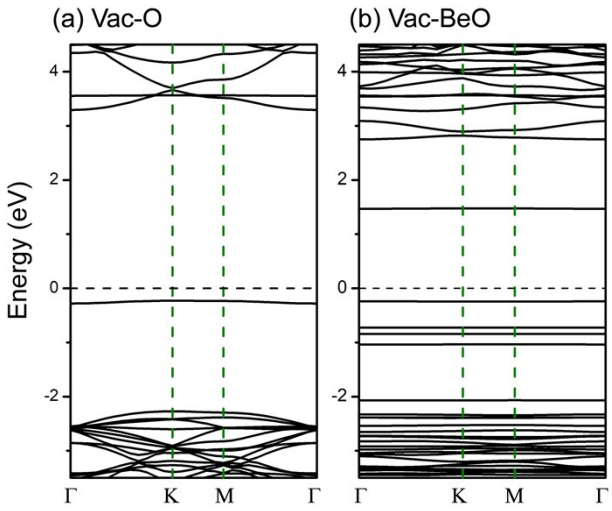


**Figure S5.** Electronic energy band structures of BeO monolayer with O single vacancy (a) and Be-O double vacancy (b).

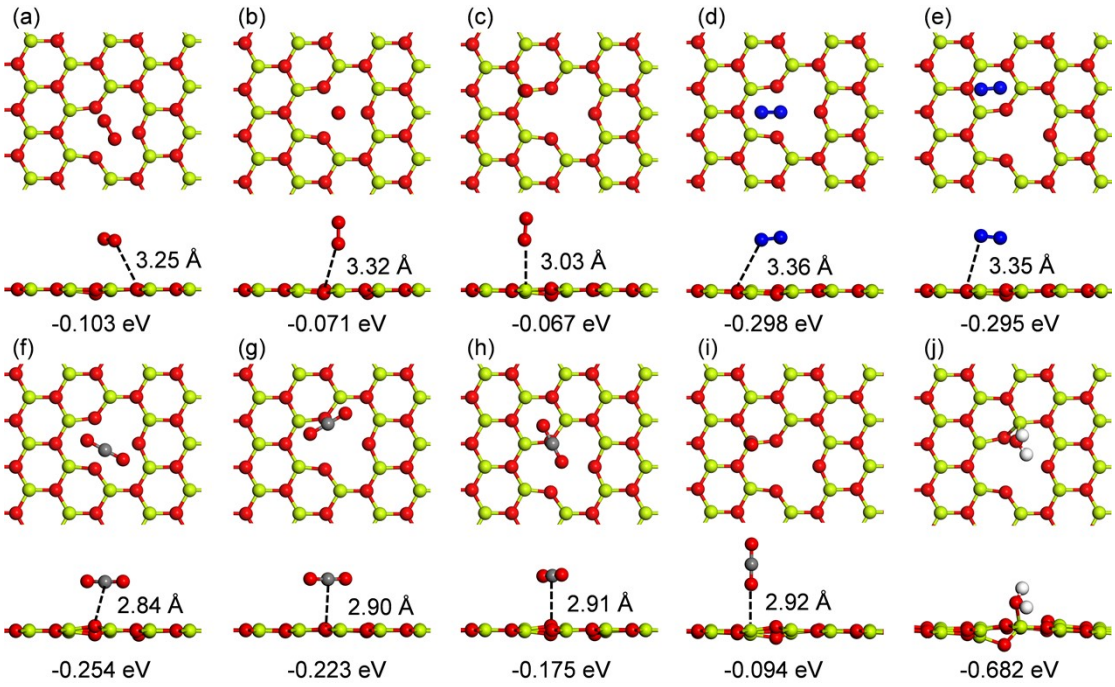


**Figure S6.** Top and side views of other possible structures for gas molecules on BeO monolayer with Be vacancy ($V_{Be}$). (a) – (c): $O_2$ on BeO monolayer with $V_{Be}$. (d) – (e): $N_2$ on BeO monolayer with $V_{Be}$. (g) – (i): $CO_2$ on BeO monolayer with $V_{Be}$. (j): $H_2O$ on BeO monolayer with $V_{Be}$. The red, green, white, gray and blue balls represent O, Be, H, C and N atoms, respectively. The shortest distance between the molecule and BeO layer is given indicated by dashed lines. The adsorption energy was given below each structure.

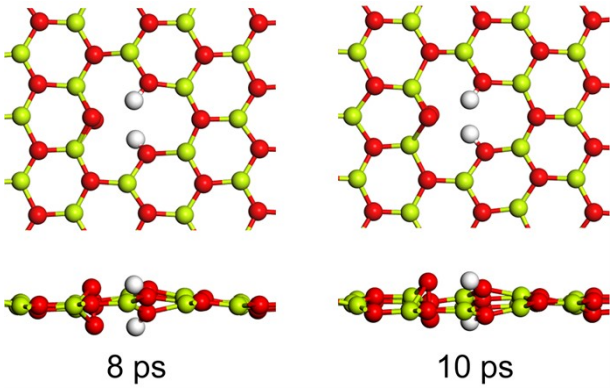


**Figure S7.** Snapshot structures of BeO monolayer with dissociated water adsorption on one Be vacancy. The red, green and white balls represent O, Be and H atoms, respectively.

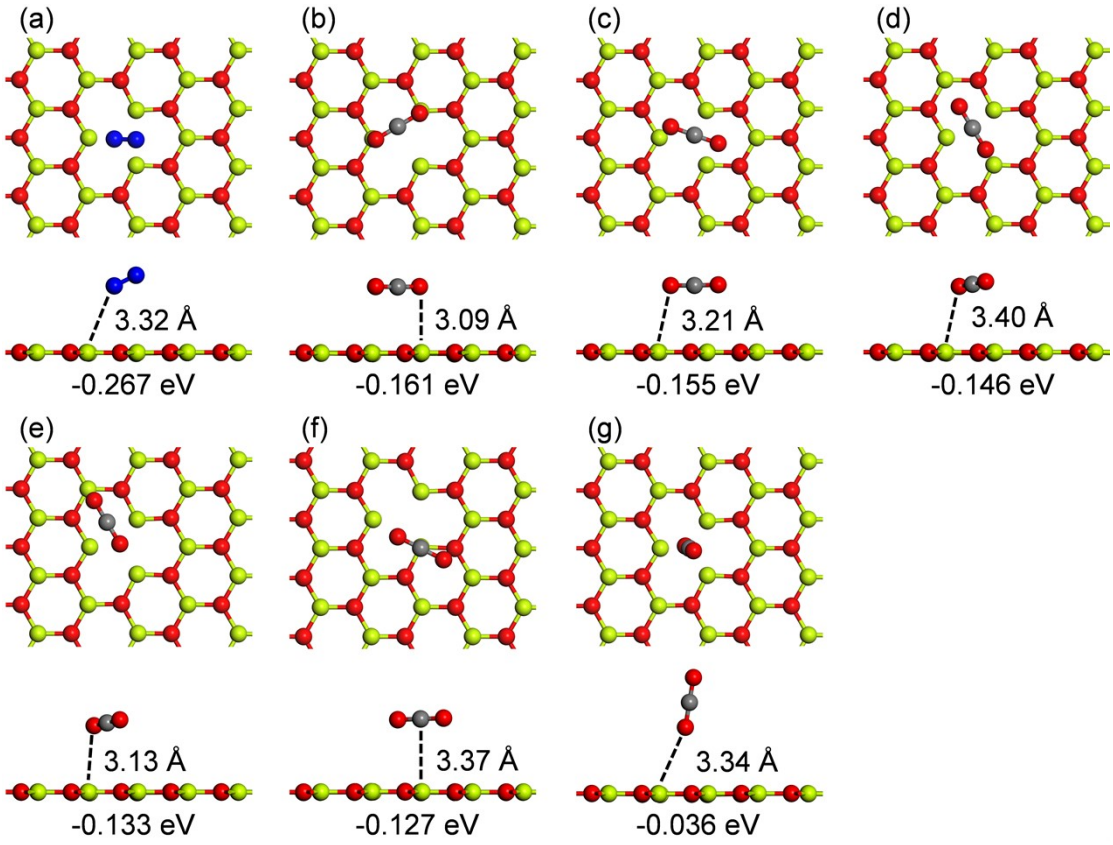


**Figure S8.** Top and side views of possible structures for gas molecules on BeO monolayer with O vacancy ($V_O$). (a): $N_2$ on BeO monolayer with $V_O$. (b) – (g) $CO_2$ on BeO monolayer with $V_O$. The red, green, gray and blue balls represent O, Be, C and N atoms, respectively. The shortest distance between the molecule and BeO layer is given indicated by dashed lines. The adsorption energy was given below each structure.