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

Supplementary Material for First-principles calculations of BeO monolayer with chemical functionalization

Hanlu Liu, Kehan Feng, Haiming Lu*, Xiangkang Meng

College of Engineering and Applied Sciences, Jiangsu Key Laboratory of Artificial Functional Materials, Collaborative Innovation Center of Advanced Microstructures, Nanjing University, Nanjing 210093, China

** Correspondence:haimlu@nju.edu.cn(H.Lu)*

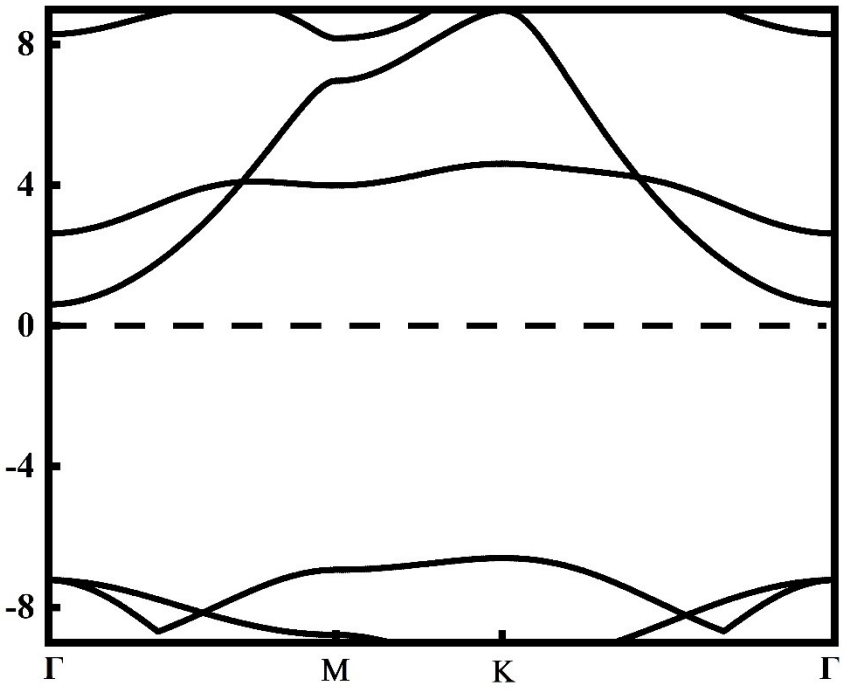

Fig. S1. Band structure of BeO monolayer by the hybrid functional HSE06.

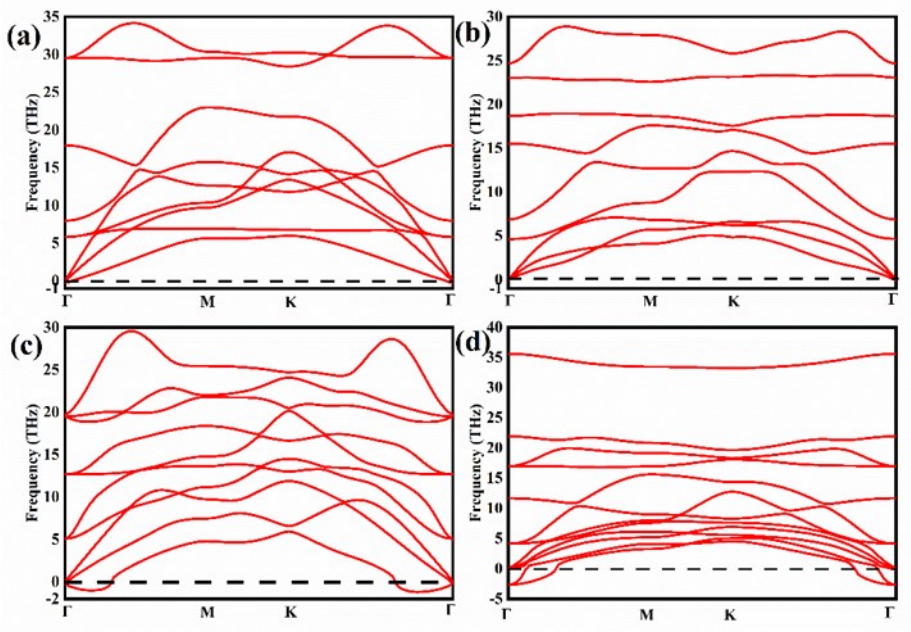

Fig. S2. The phonon spectrums of the most stable adsorption configurations for (a) half-hydrogenation, (b) half-fluorination, (c) full-hydrogenation, and (d) full-fluorination.

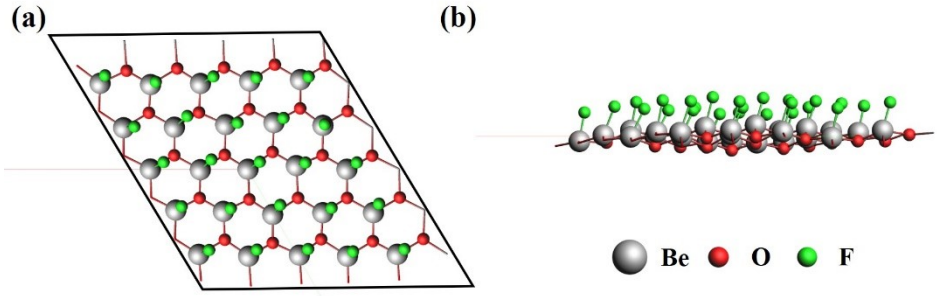

Fig. S3. Top (a) and side (b) views of AIMD simulation results for 5×5 BeO supercell after the half-fluoridation at T_B.

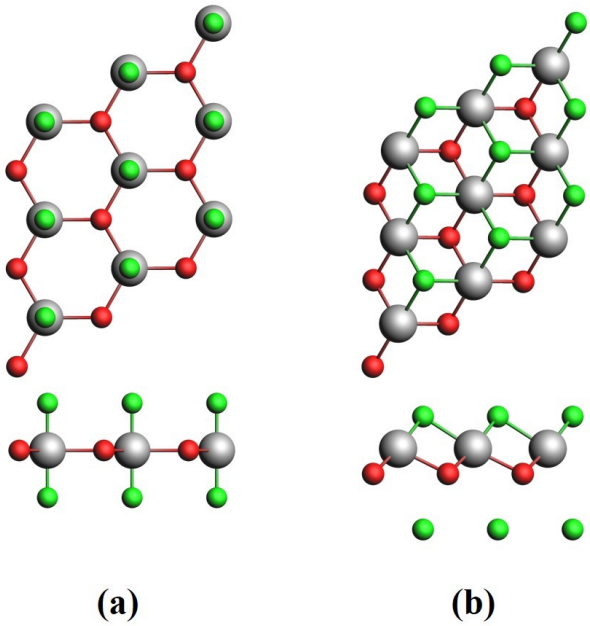

Fig. S4. Top and side views of optimized BeO monolayer after full-fluoridation at (a) T_{Be2} and (b) T_{C2} sites.