

# Crown ethers in hydrogenated graphene

*Kai Guo,<sup>a</sup> Sitong Liu,<sup>a</sup> Haoming Tu,<sup>b</sup> Zhikun Wang,<sup>b</sup> Liang Chen,<sup>a</sup> Haiqing Lin,<sup>c</sup>*

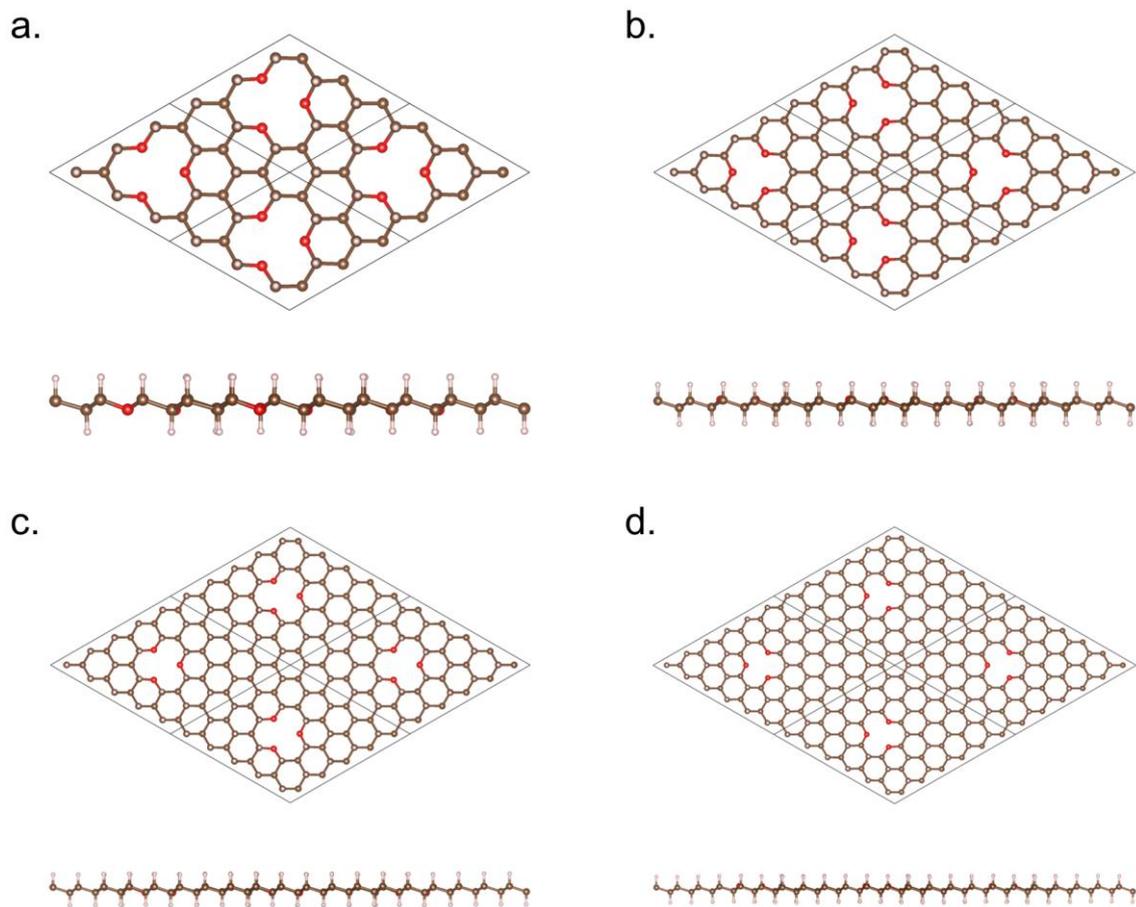
*Maosheng Miao,<sup>d</sup> Jing Xu,<sup>\*a</sup> Wei Liu,<sup>\*a</sup>*

a Department of Optical Engineering, Zhejiang A&F University, Hangzhou, Zhejiang,  
311300, P. R. China

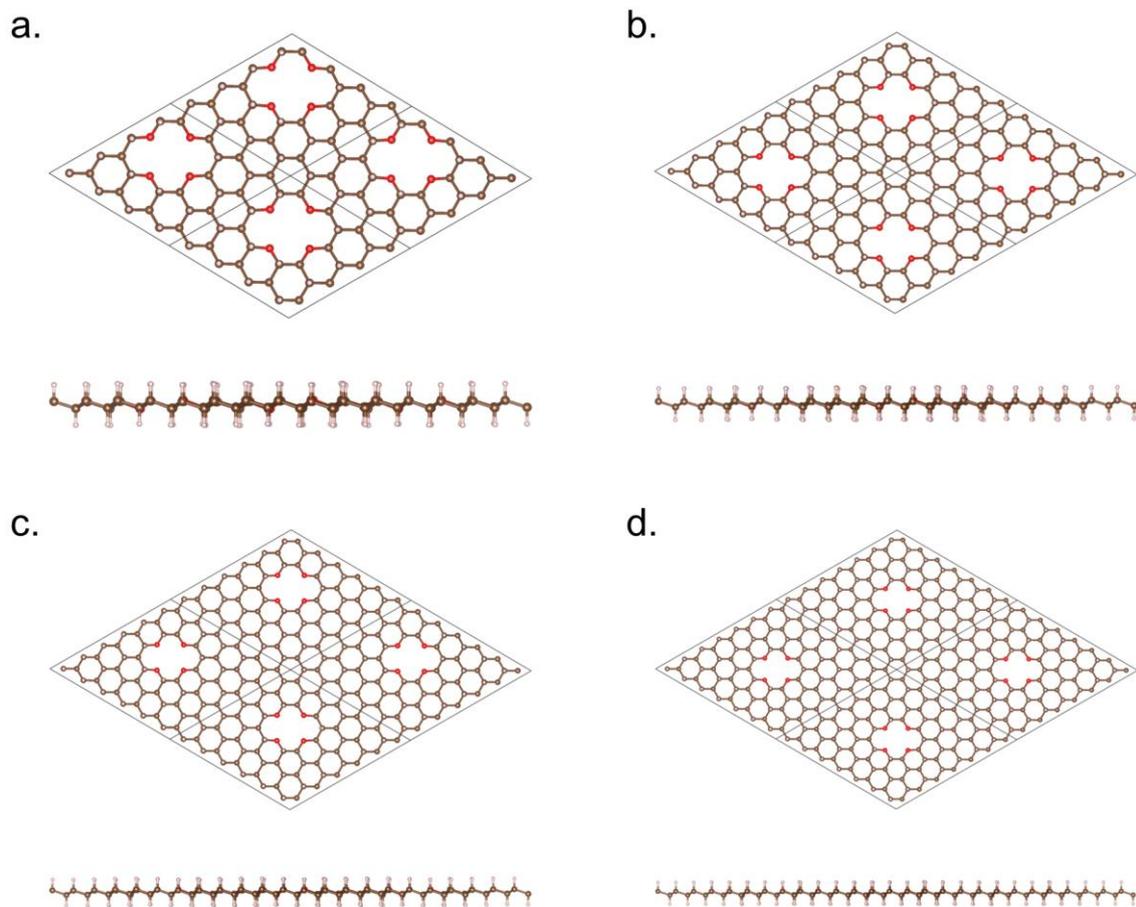
b Department of Chemistry, Zhejiang A&F University, Hangzhou, Zhejiang, 311300,  
P. R. China

c Beijing Computational Science Research Center, Beijing, 100193, P. R. China

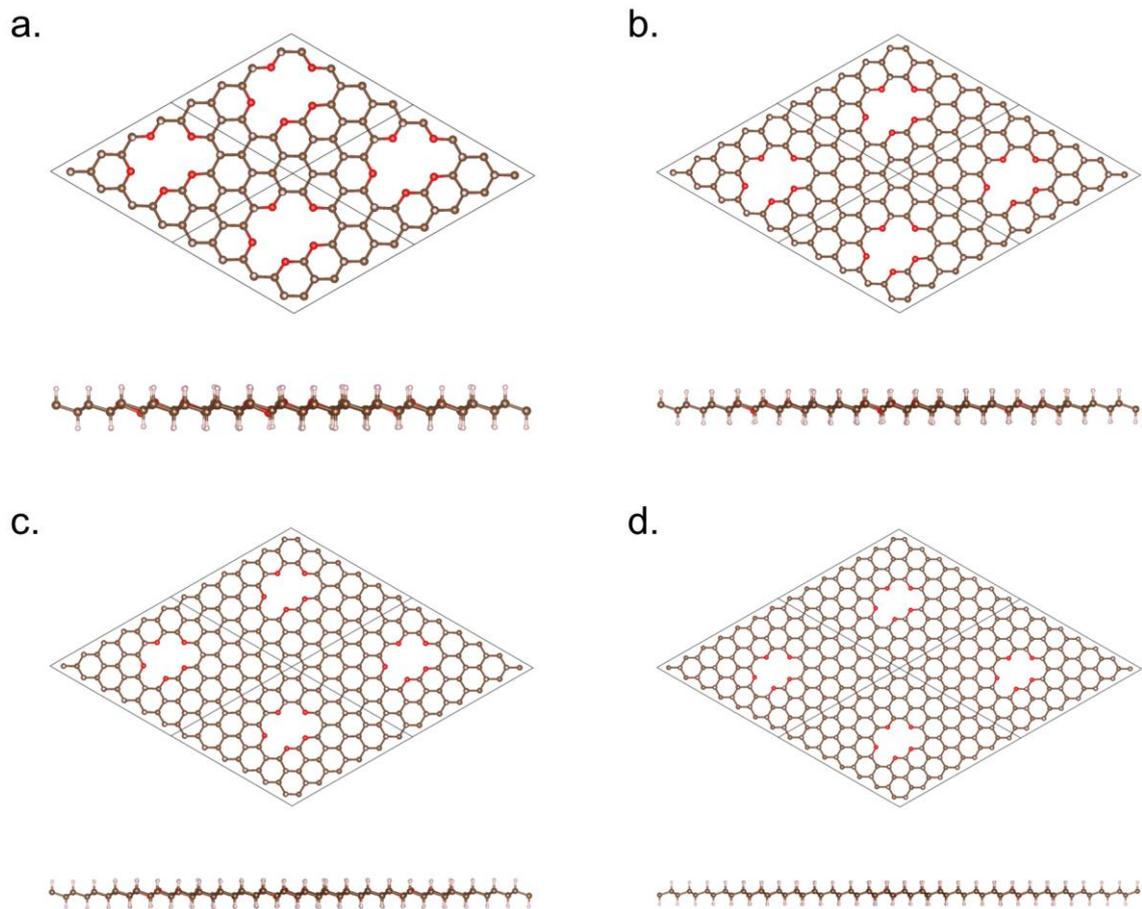
d Department of Chemistry & Biochemistry, California State University, Northridge,  
CA, 91330-8262, USA



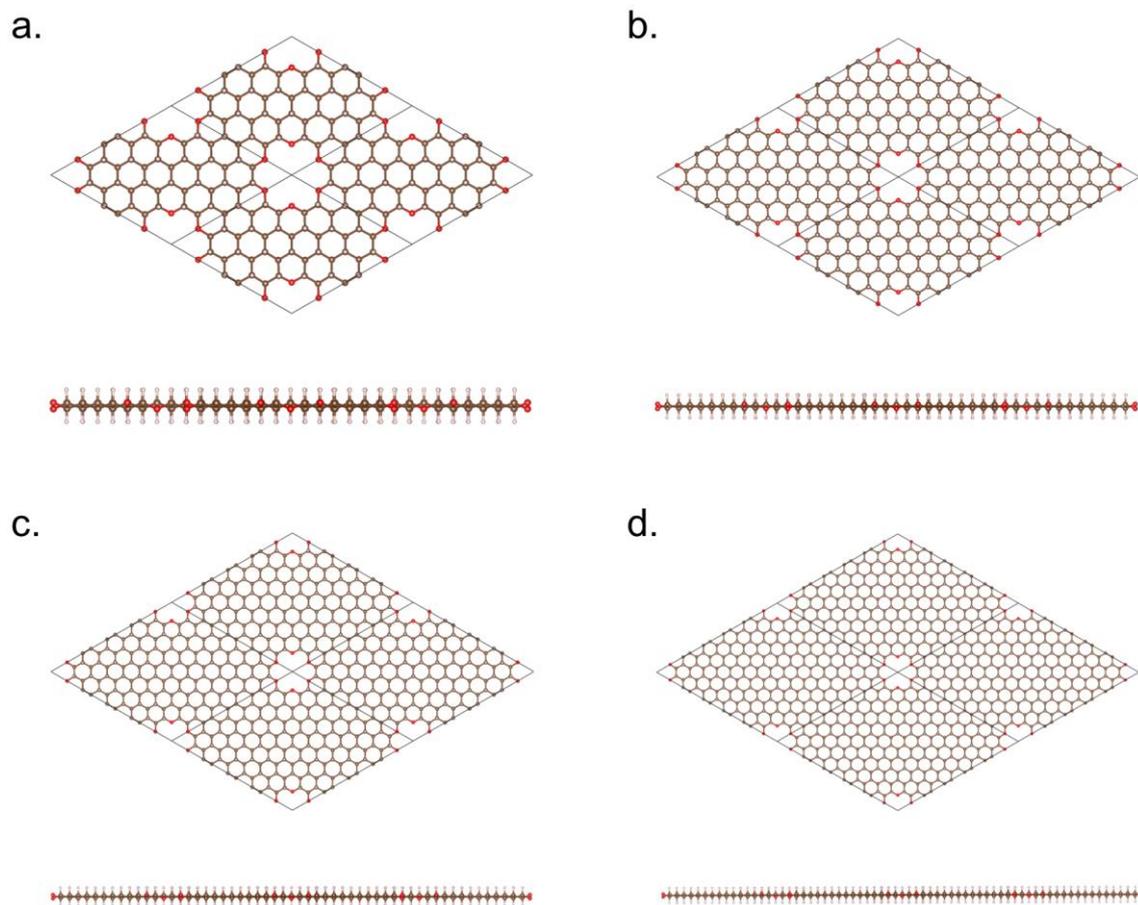
**Figure S1.** Top and side views of the optimized structures of (a) crown-3-2, (b) crown-3-3, (c) crown-3-4 and (d) crown-3-5.



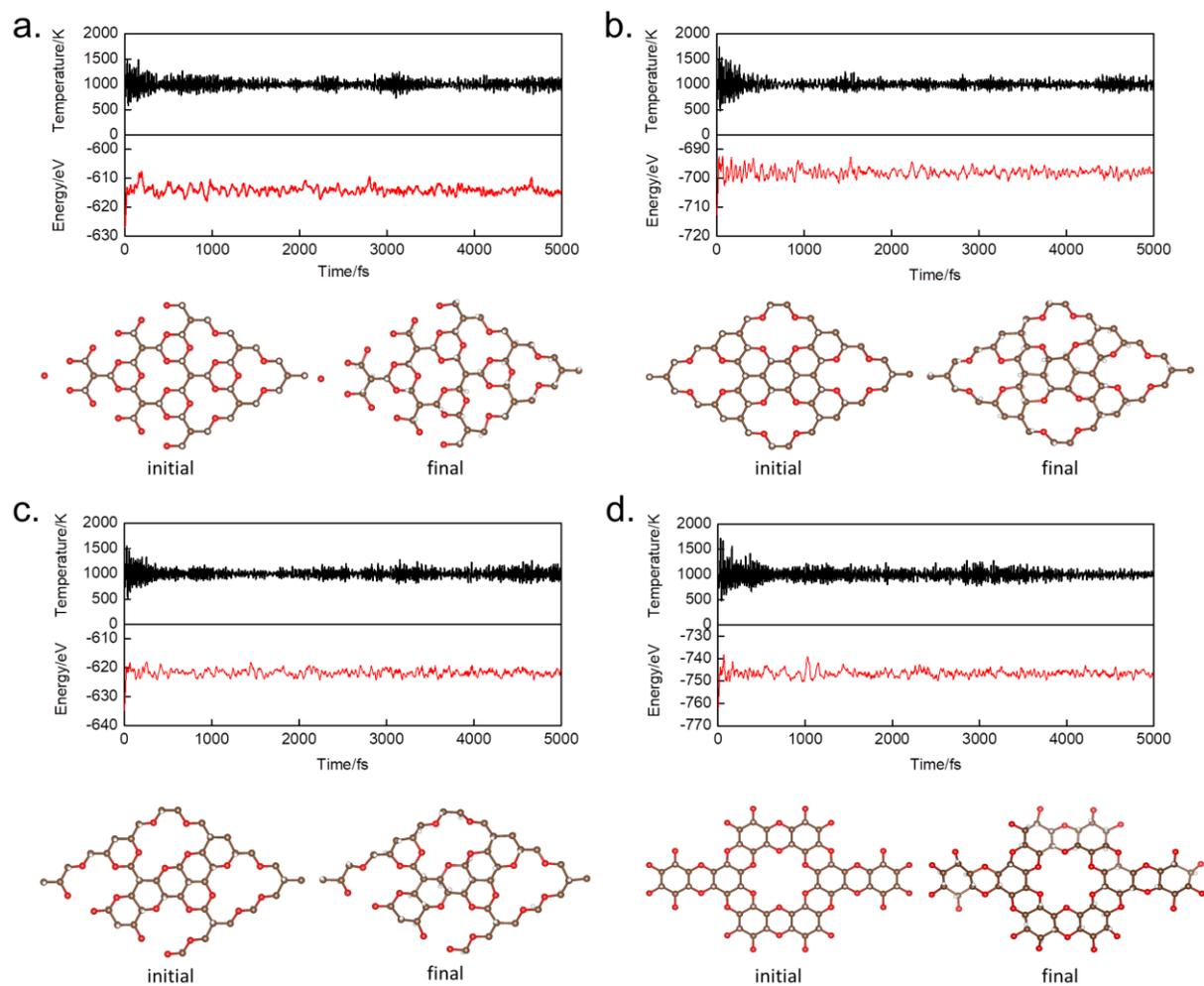
**Figure S2.** Top and side views of the optimized structures of (a) crown-4-2, (b) crown-4-3, (c) crown-4-4 and (d) crown-4-5.



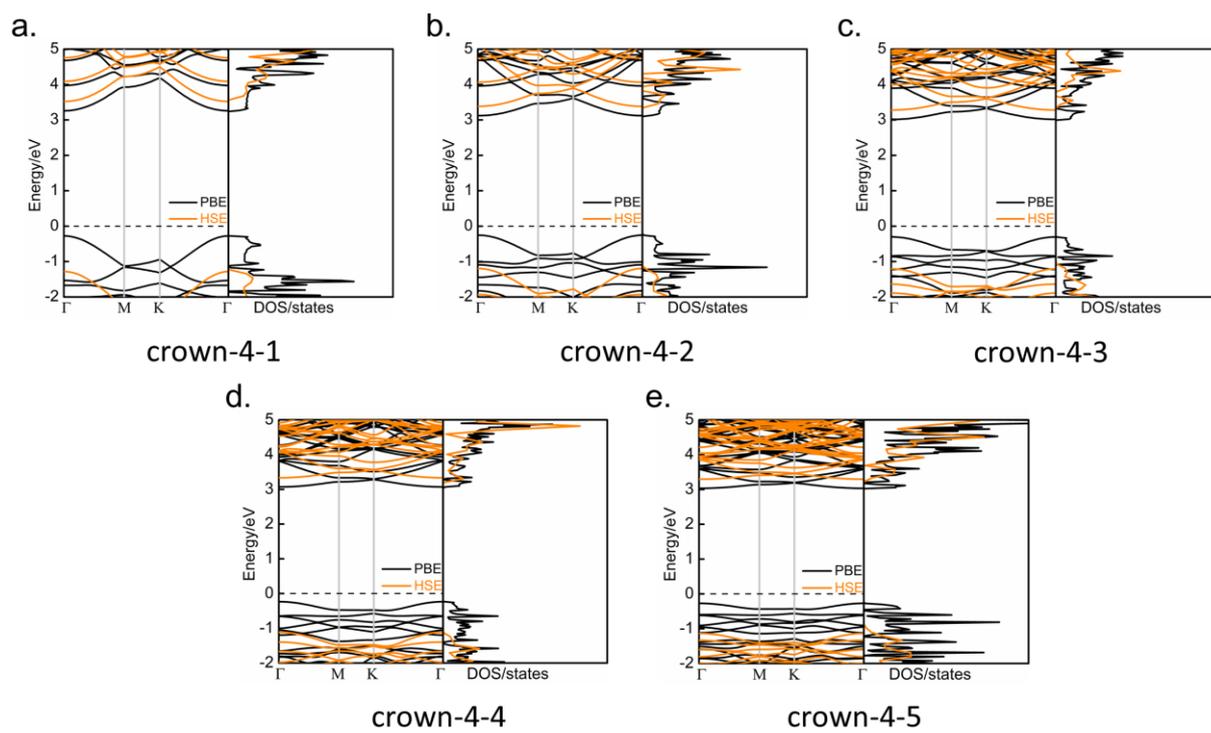
**Figure S3.** Top and side views of the optimized structures of (a) crown-5-2, (b) crown-5-3, (c) crown-5-4 and (d) crown-5-5.



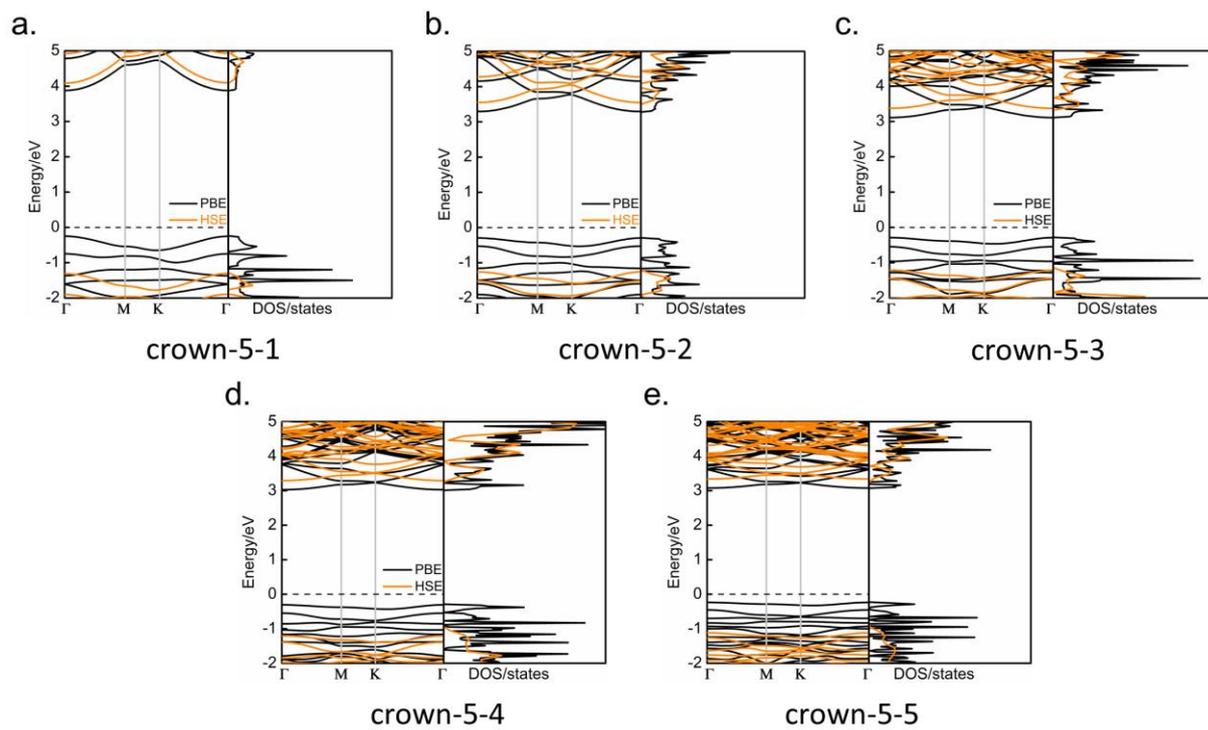
**Figure S4.** Top and side views of the optimized structures of (a) crown-6-2, (b) crown-6-3, (c) crown-6-4 and (d) crown-6-5.



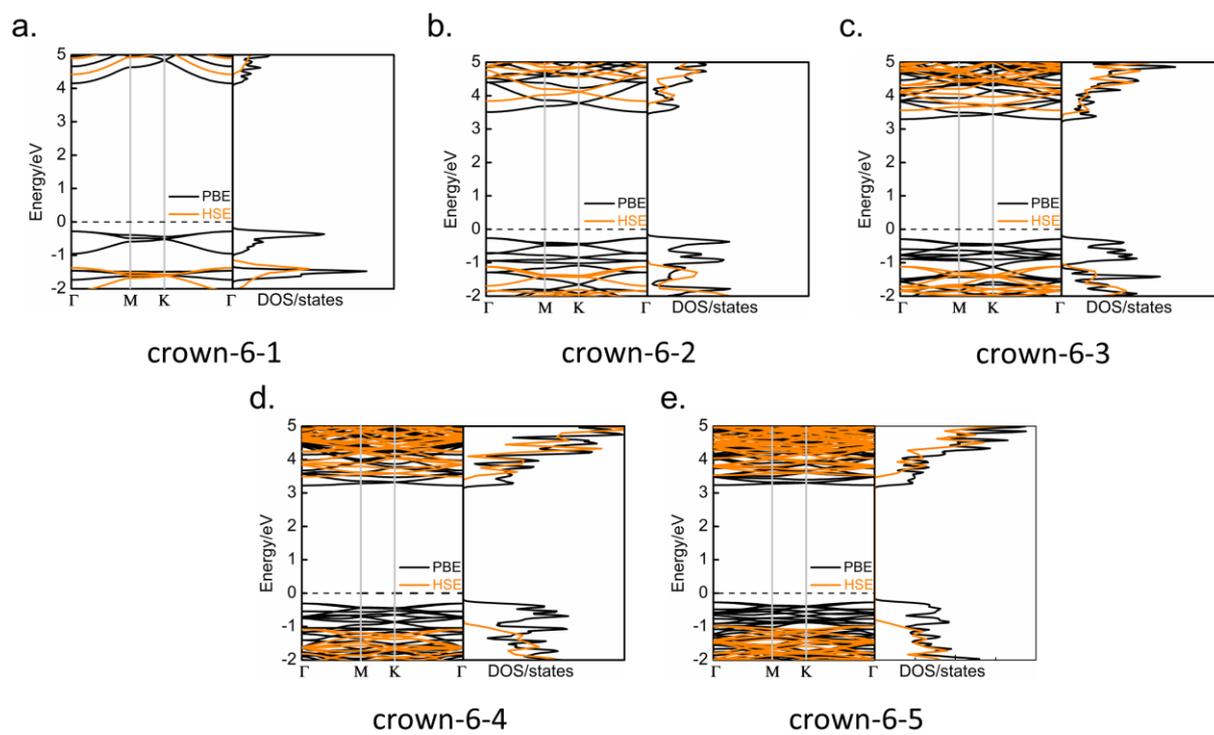
**Figure S5.** Fluctuation of temperature and energy against time for AIMD simulations at 1000K: (a) crown-3-1, (b) crown-4-1, (c) crown-5-1, (d) crown-6-1. The initial and final snapshots of the simulations are also shown.



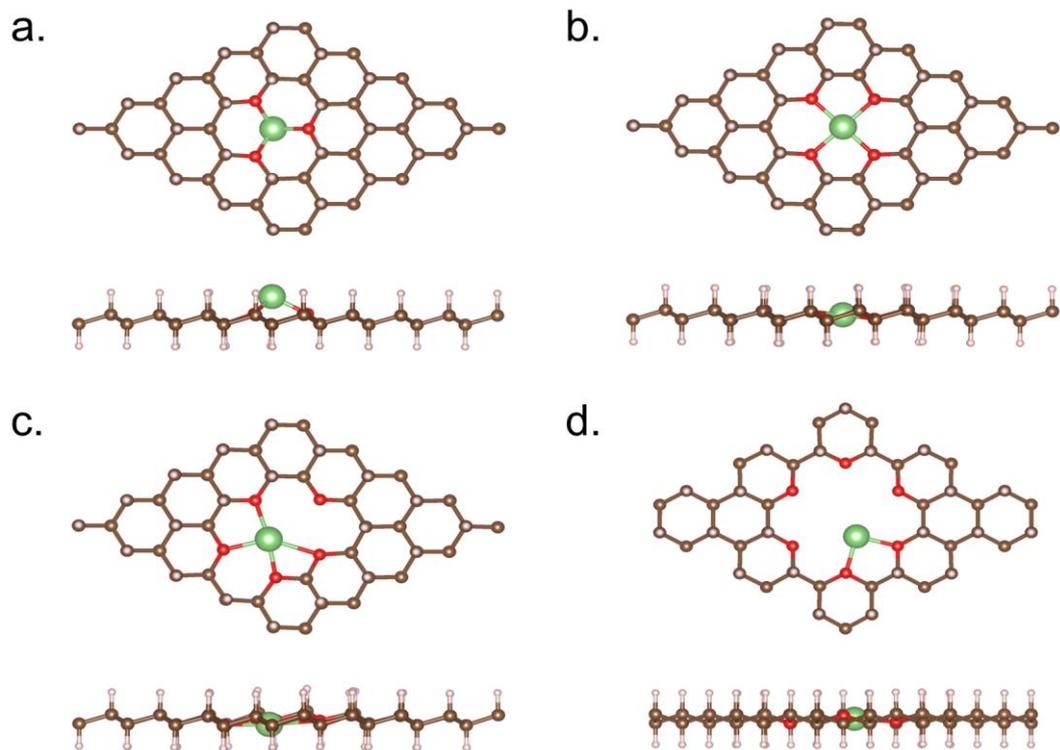
**Figure S6.** The band structures and DOS of (a) crown-4-1, (b) crown-4-2, (c) crown-4-3, (d) crown-4-4, (e) crown-4-5.



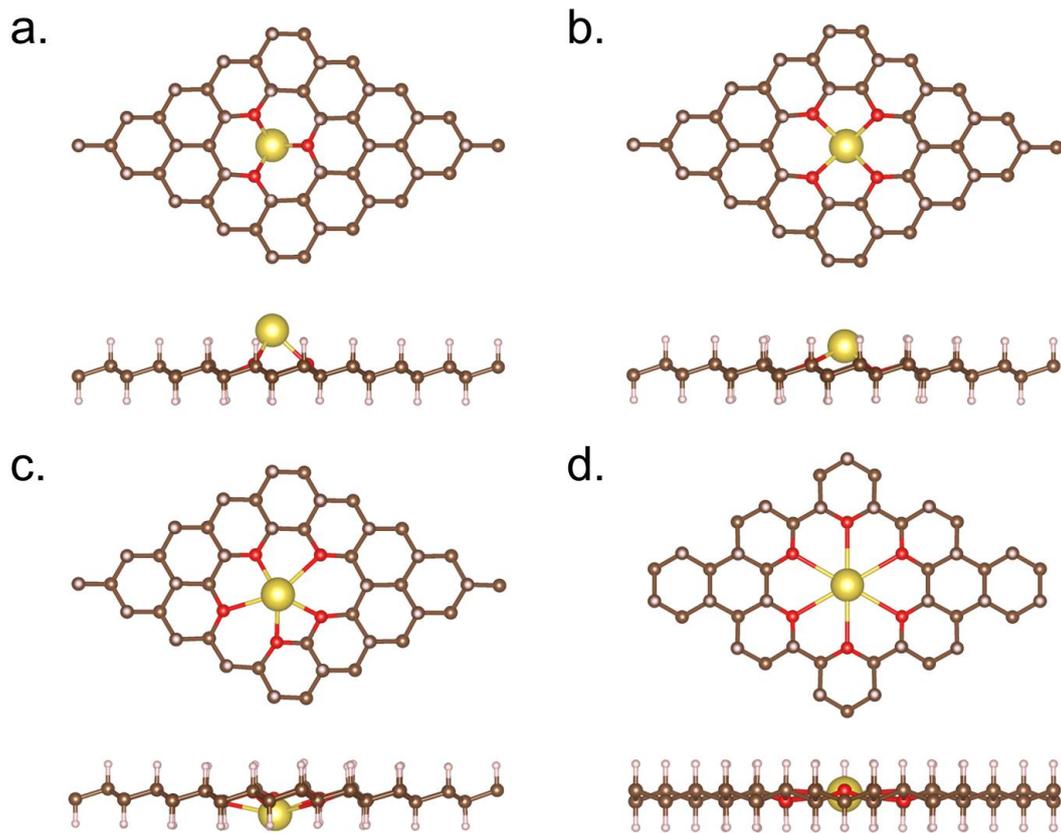
**Figure S7.** The band structures and DOS of (a) crown-5-1, (b) crown-5-2, (c) crown-5-3, (d) crown-5-4, (e) crown-5-5.



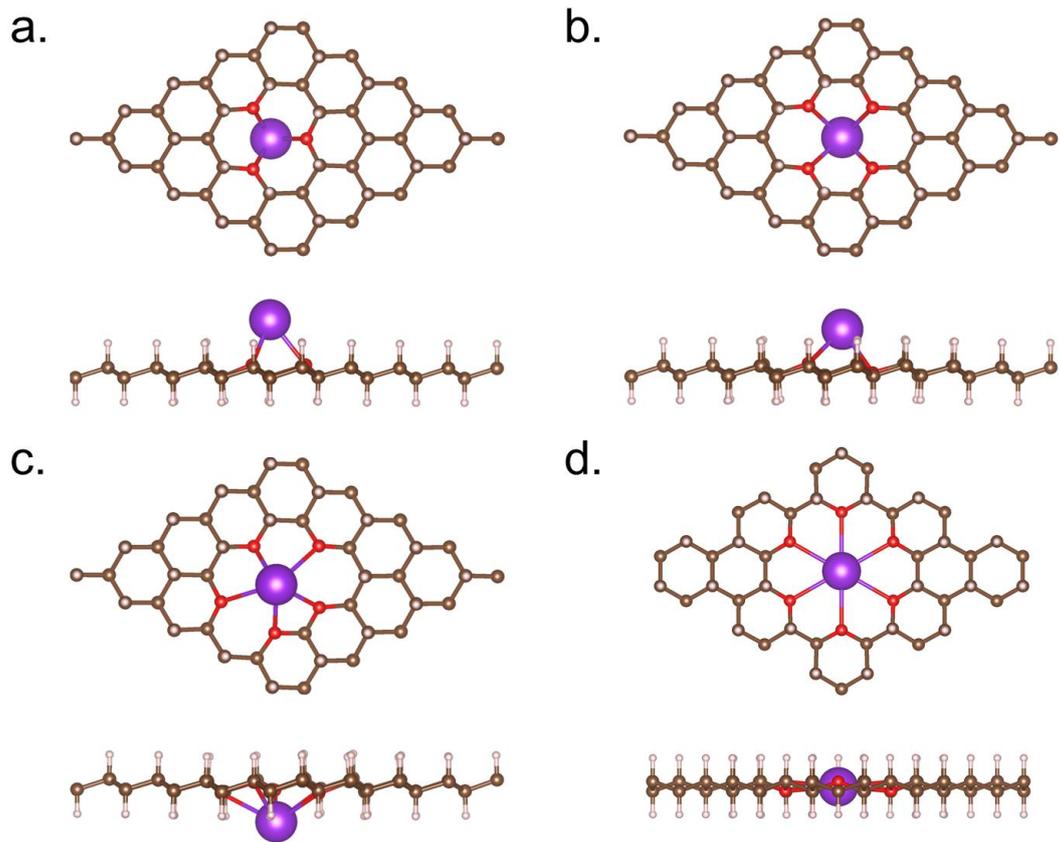
**Figure S8.** The band structures and DOS of (a) crown-6-1, (b) crown-6-2, (c) crown-6-3, (d) crown-6-4, (e) crown-6-5.



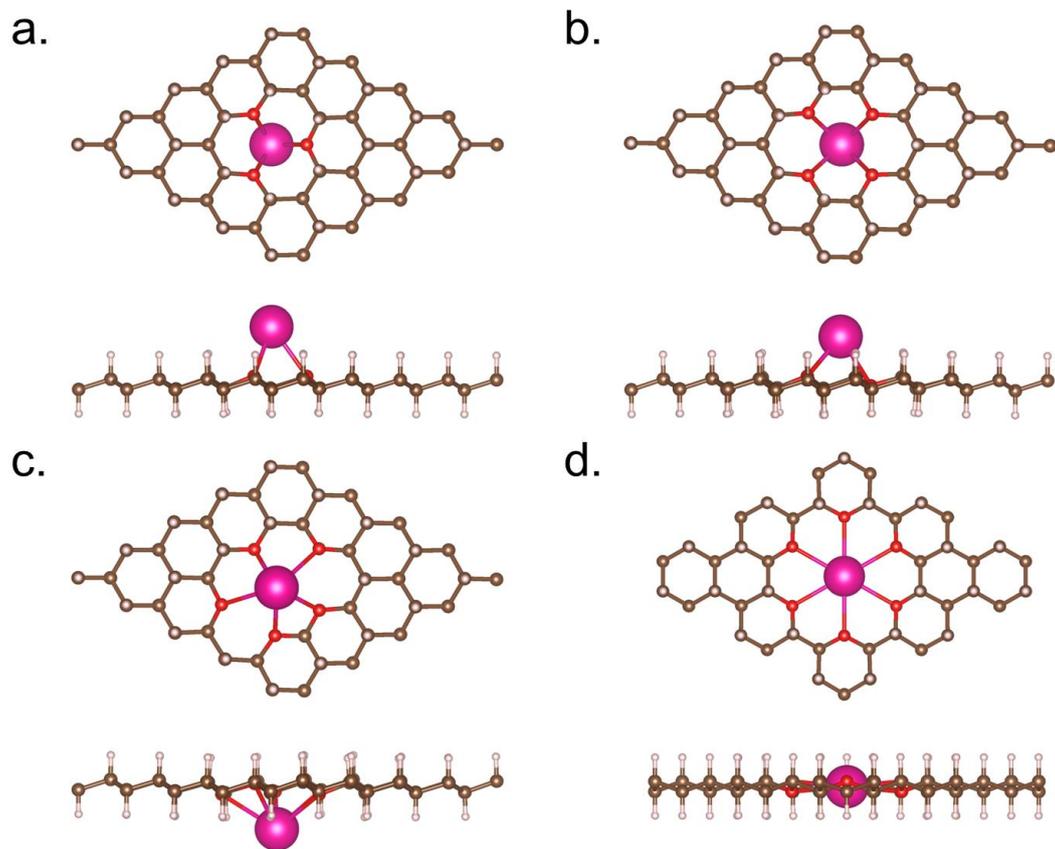
**Figure S9.** The top and side view of  $\text{Li}^+$  adsorbed by (a) crown-3-4; (b) crown-4-3; (c) crown-5-3; (d) crown-6-2.



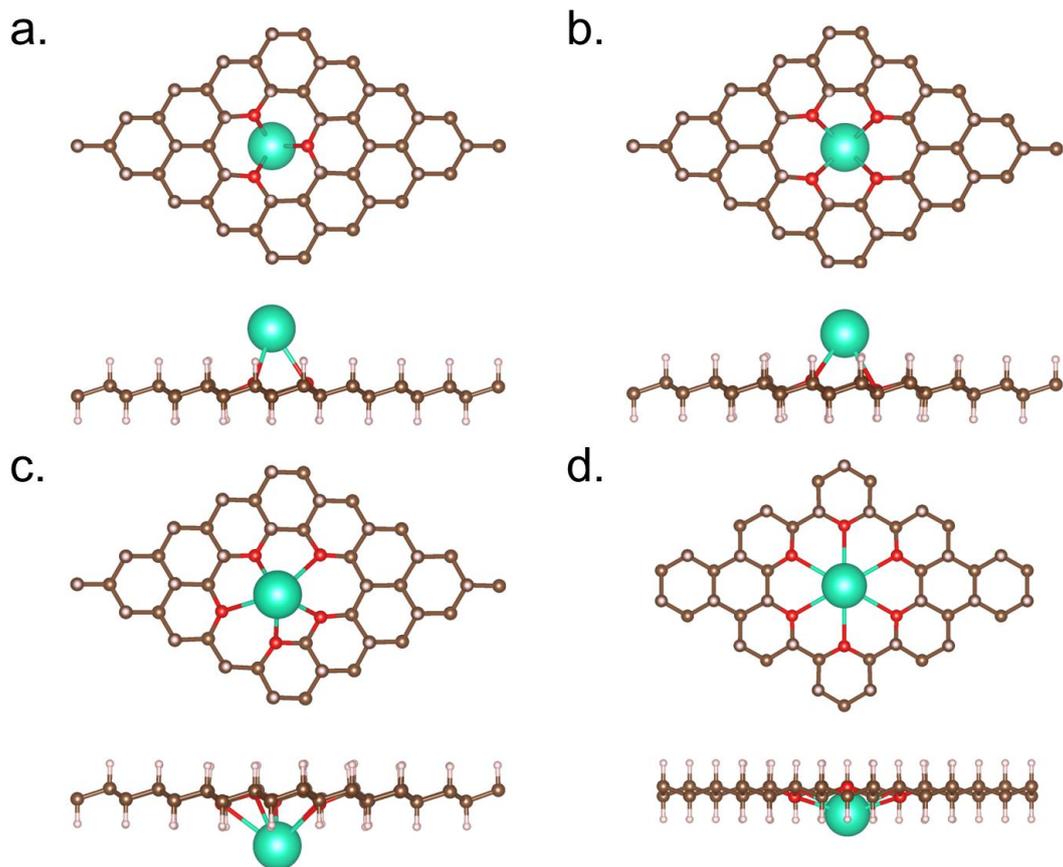
**Figure S10.** The top and side view of  $\text{Na}^+$  adsorbed by (a) crown-3-4; (b) crown-4-3; (c) crown-5-3; (d) crown-6-2.



**Figure S11.** The top and side view of  $K^+$  adsorbed by (a) crown-3-4; (b) crown-4-3; (c) crown-5-3; (d) crown-6-2.



**Figure S12.** The top and side view of  $\text{Rb}^+$  adsorbed by (a) crown-3-4; (b) crown-4-3; (c) crown-5-3; (d) crown-6-2.



**Figure S13.** The top and side view of  $\text{Cs}^+$  adsorbed by (a) crown-3-4; (b) crown-4-3; (c) crown-5-3; (d) crown-6-2.