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

Supporting Information

Machine-learning-assisted discovery of boron-doped graphene with high work function as anode material for Li/Na/K-ion batteries

Yi Luo,[a] Haiyuan Chen,[*a] Jianwei Wang [a] and Xiaobin Niu [a]

[a]*School of Materials and Energy, University of Electronic Science and Technology of China, Chengdu 610054, P.R. China*

[*]Corresponding author: hychen@uestc.edu.cn

Table.S1. Size of configuration space (N_{conf}) and the number of structures (N_{data}) in data set at different doping number (n_B)

n_B	4	5	6	7	8	9	10
N_{conf}	241	1129	5002	17929	55817	147362	338741
N_{data}	2	4	18	64	198	521	1197

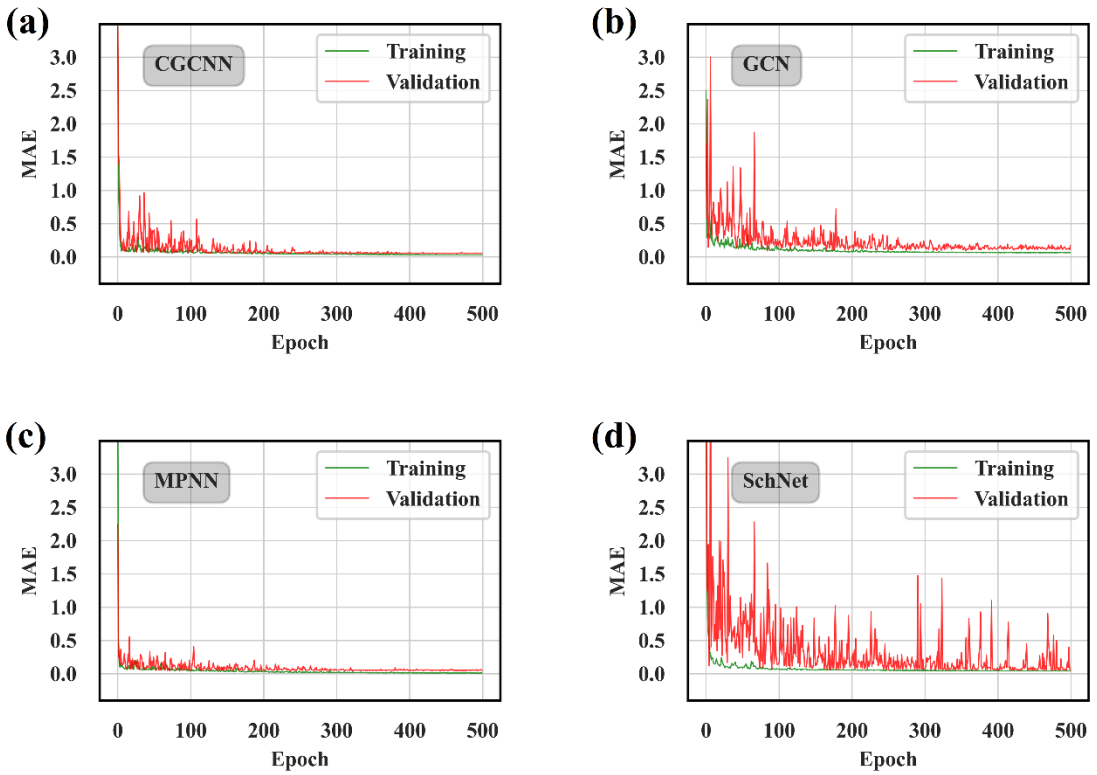

Fig. S1. Training/validation MAE of (a) CGCNN, (b) GCN, (c) MPNN, and (d) SchNet models.

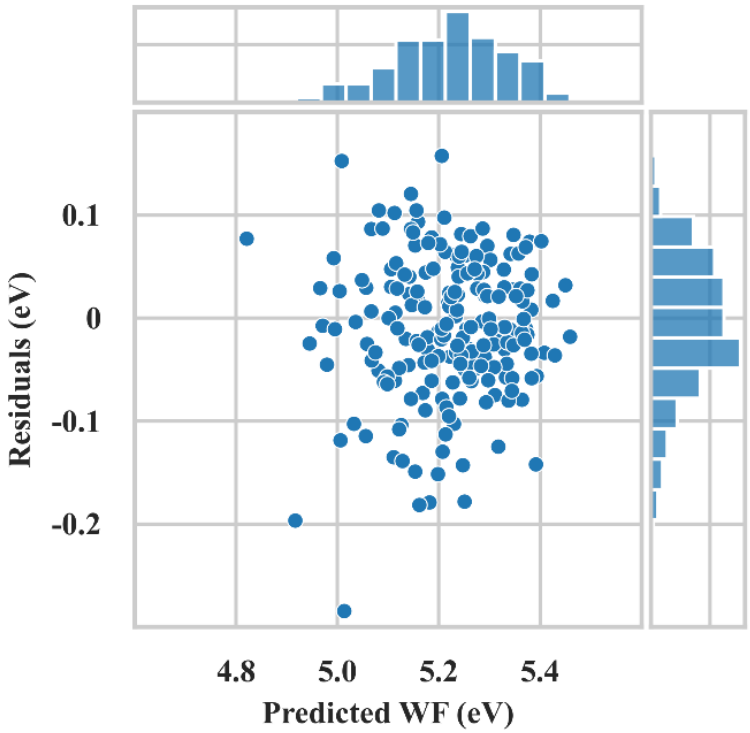

Fig. S2. Residuals distribution of the test data set achieved by the CGCNN model.

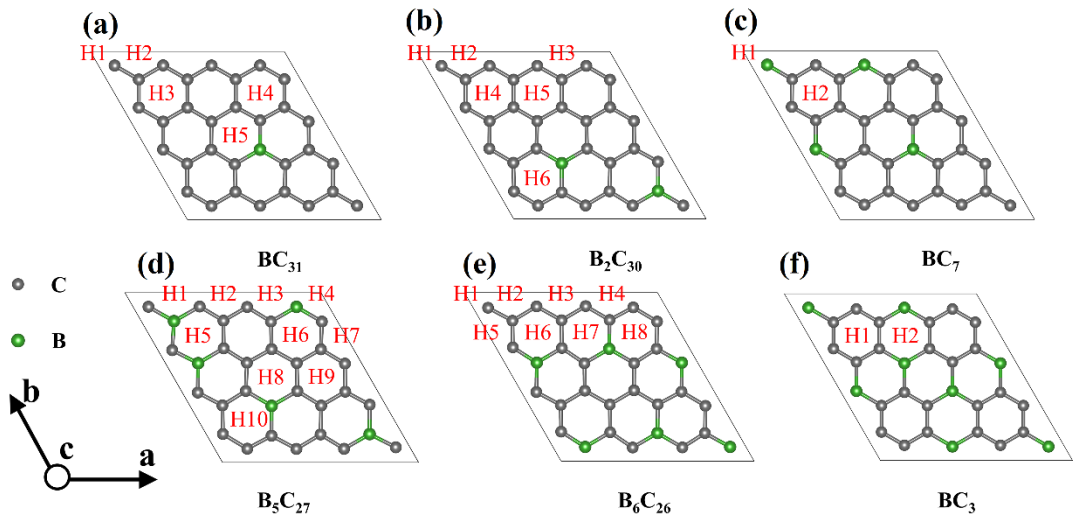

Fig. S3. Crystal structures of (a) BC_{31}, (b) B_2C_{30}, (c) BC_7, (d) B_5C_{27}, (e) B_6C_{26}, and (f) BC_3. The hollow sites for alkali metal adsorption are marked with red color.

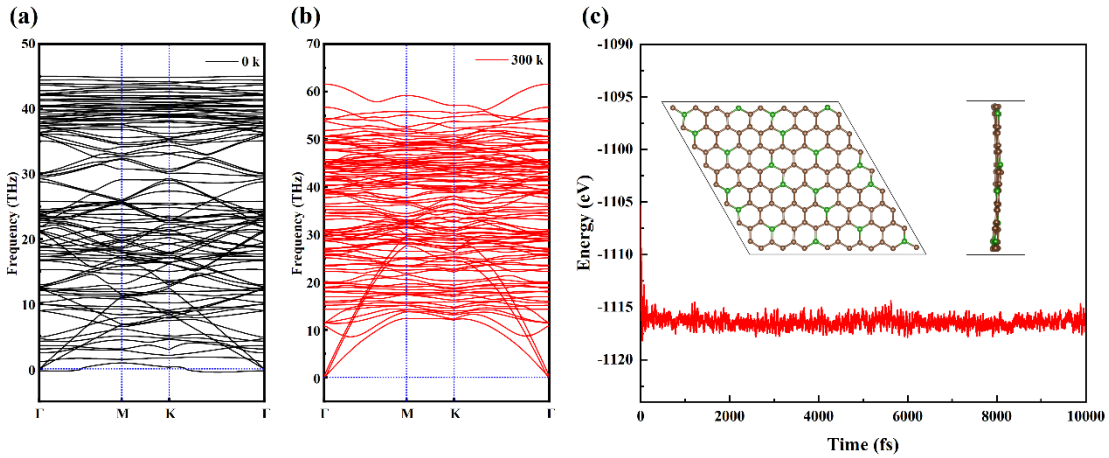

Fig. S4. Phonon spectra of B_5C_{27} at (a) 0 K and (b) 300 K. (c) The energy oscillation of $B_{20}C_{108}$ in AIMD simulation, and the insets are the top and side views of final snapshot after AIMD simulations for 10 ps at 300 K, with a time step of 1 fs.

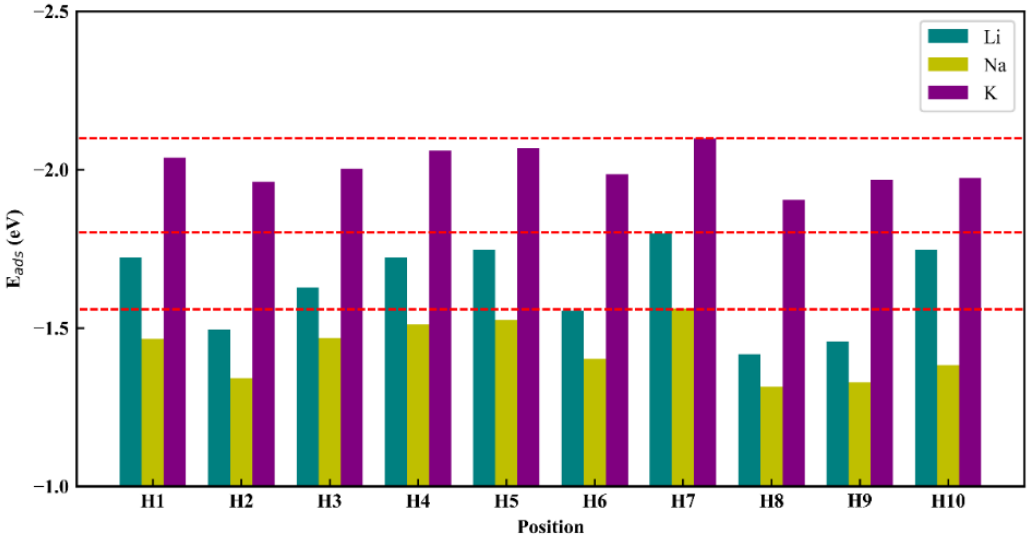

Fig. S5. E_{ads} of Li/Na/K on different hollow sites in B_5C_{27}.

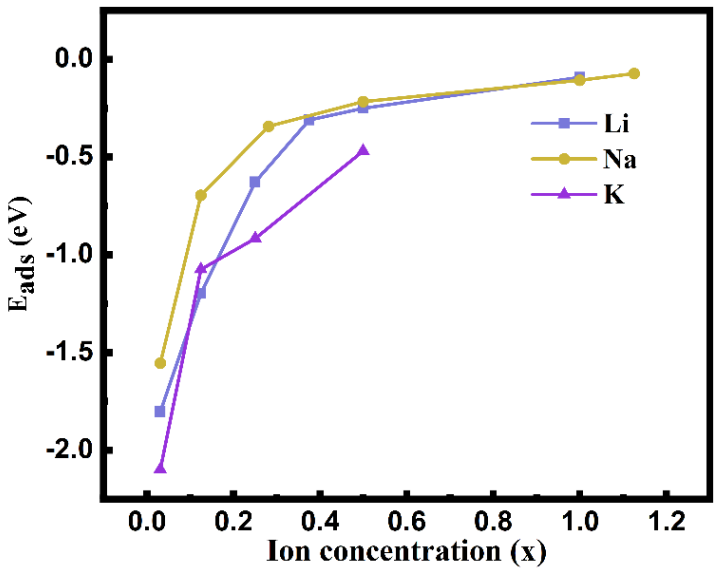

Fig. S6. Adsorption energy as a function of the concentrations of Li/Na/K adatoms.

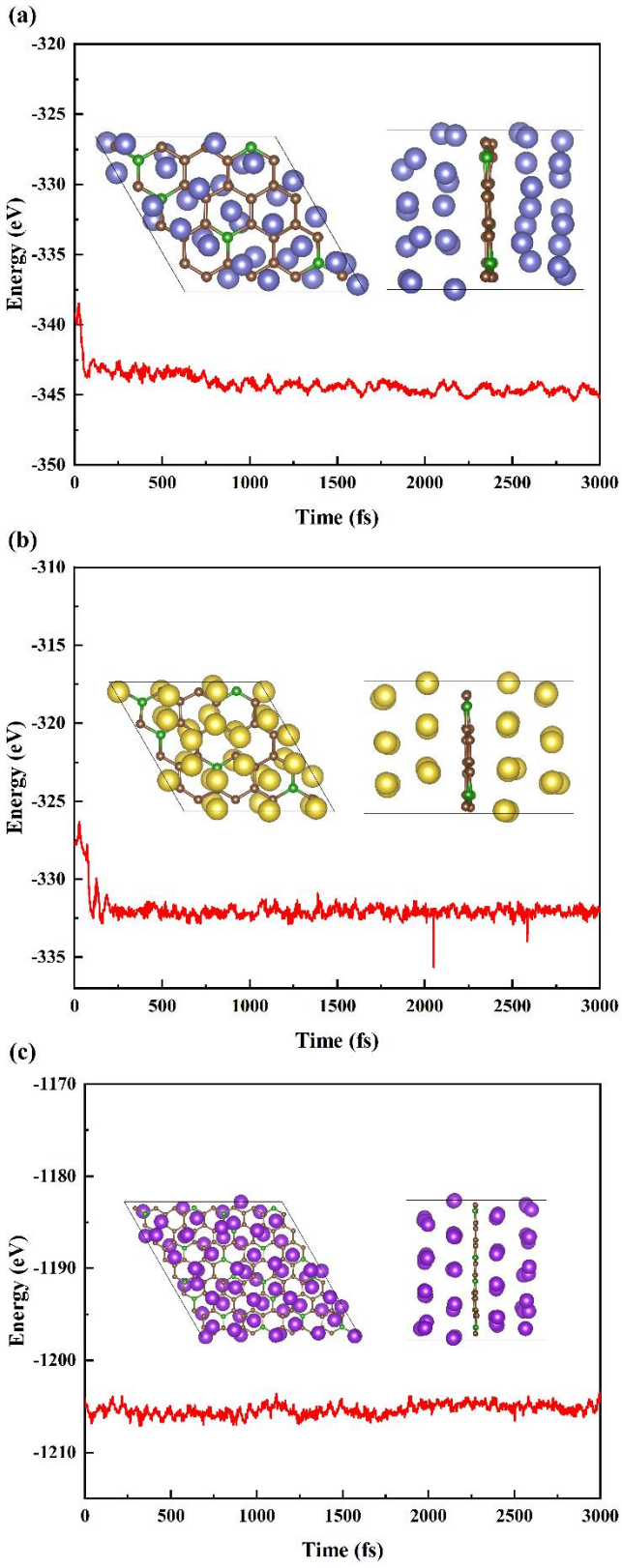

Fig. S7. The results of AIMD simulations of (a) $B_5C_{27}Li_{32}$, (b) $B_5C_{27}Na_{36}$, and (c) $B_{20}C_{108}K_{64}$. The insets are the top and side views of final snapshot after AIMD simulation for 3 ps at 300 K, with a time step of 1 fs.