Supporting information

A Novel BC_2N monolayer as anode material for Li-ion battery

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Computational Methods

The density functional theory (DFT) calculations were carried out using the VASP code [1]. The electron-ion interaction was described using the projector-augmented wave (PAW)[2]. We used the generalized gradient approximation (GGA) in Perdew-Burke-Ernzerhof functional (PBE) to describe the exchange-correlation functional [3-4]. To take the van der Waals interactions into account, the D2-Grimme dispersion correction[5] was used. We used a plane-wave energy cutoff of 500 eV for all the calculations. To reduce the artificial interactions between neighboring layers, we employed a large vacuum slab (~26 Å) along the z-direction. We employed a Gaussian smearing technique with a small SIGMA value of 0.05 for all our calculations. For geometric optimization, we use 12×12×1 Γ-centered k-meshes. The cell's volume, shape, and all of its atoms were completely relaxed until the residual force was less than 0.01 eV/Å. The electronic structure and optical characteristics of BC_2N monolayer were acquired using the Heyd, Scuseria and Ernzerhof functional(HSE06)[6]. For 3D band structure calculation, we used 40×40×1 Γ-centered k-meshes. To obtain detailed and accurate phonon spectra data for BC_2N, we utilized the density functional perturbation theory (DFPT) method in conjunction with the Phonopy software package[7]. We used a 4×4×1 supercell of BC_2N for phonon spectra calculation. To further analyze the bonding properties of BC_2N, crystal orbital Hamilton population (COHP) calculations were performed using the lobster code[8]. We use a 3×3×1 supercell of BC_2N monolayer to perform the Ab initio molecular dynamics (AIMD) simulations. The Nose-Hoover method was used to solve the ionic motion equations. The time step of AIMD simulation is set to be 1.0 fs. We equilibrated the system at 300, 450 and 600 K for 10 ps in canonical ensemble (NVT). The climbing image nudged elastic bond (CI-NEB) method[9] was utilized to explore the pathways and energy barriers associated with the diffusion of Li in the given system, which yielded important information about the underlying mechanism and kinetics of Li diffusion. We used Vaspkit code to derive the mechanical and optical properties of BC_2N monolayer from the raw VASP calculation results [10].

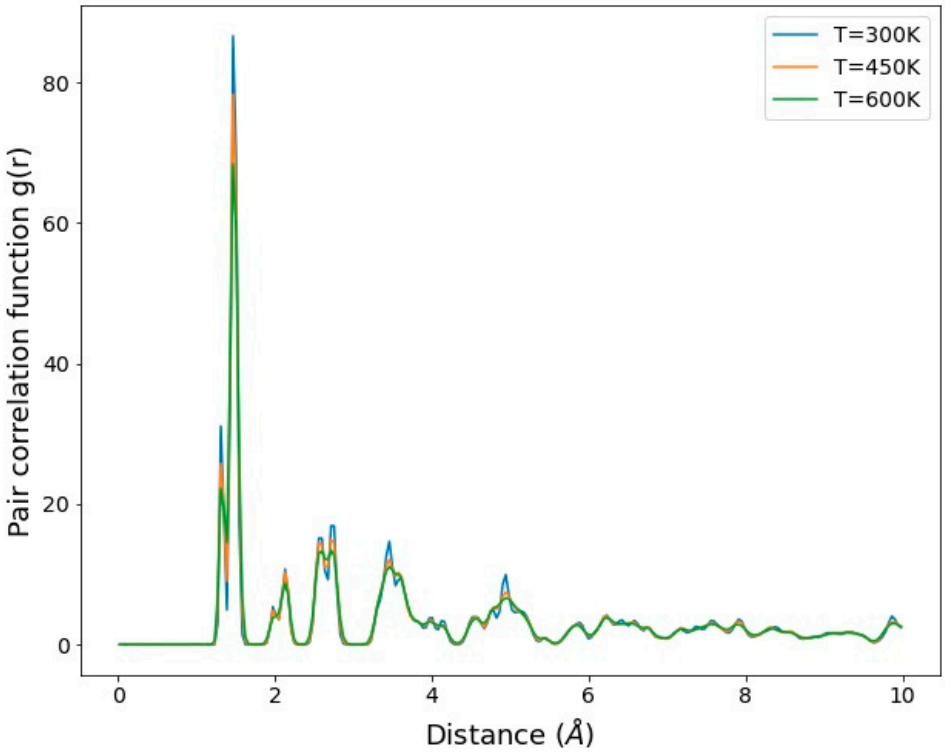

Figure S1 Pari correlation function of BC2N monolayer.

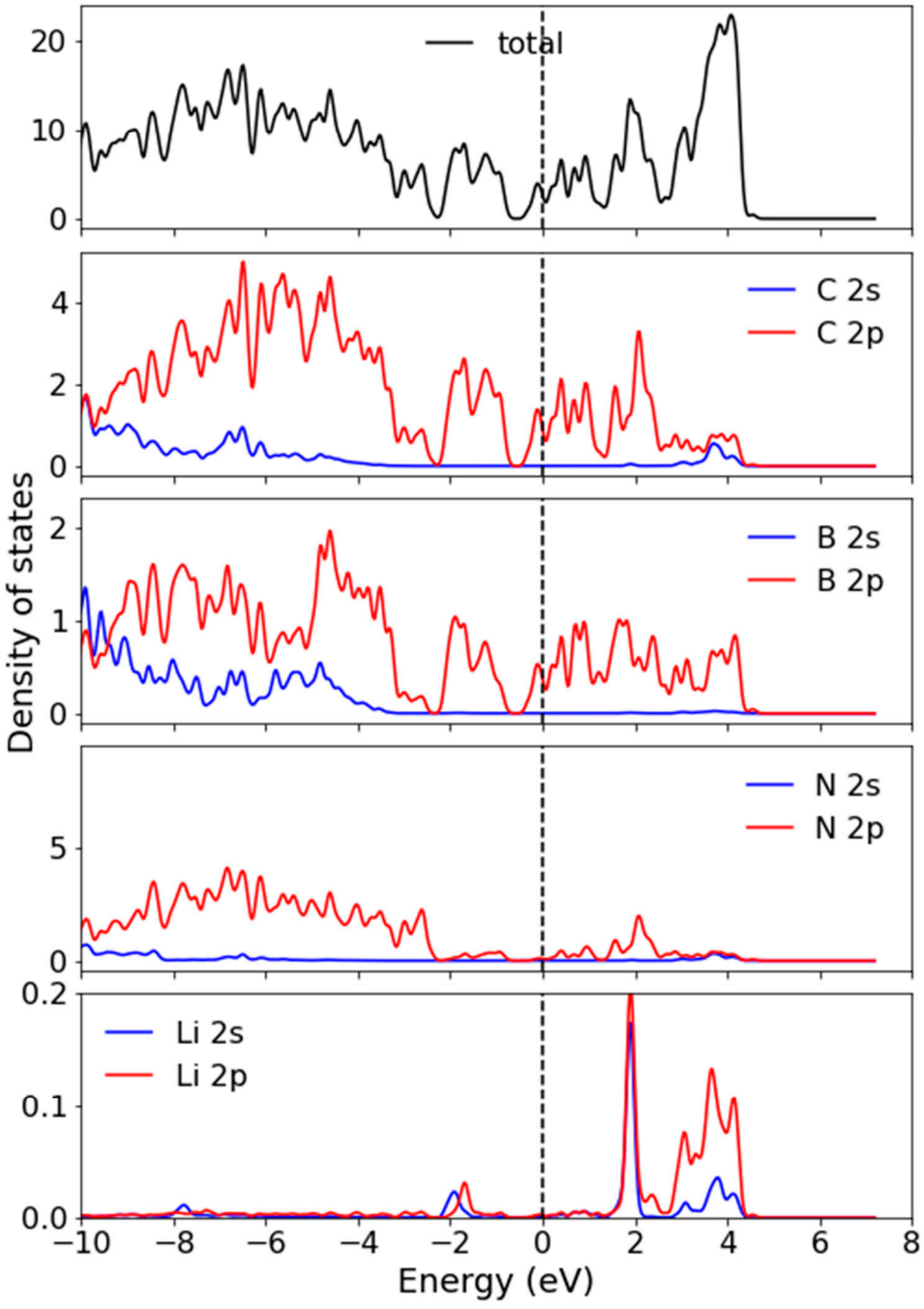

Figure S2 The density of state of Li adsorb on BC2N monolayer.

Table S1 The -ICOHP value for the C1-C2, C-B, C-N and N-B bonds.

C1-C2 (eV)	C-B (eV)	C-N (eV)	B-N (eV)
8.78	8.25	12.09	7.54

Table S2 Bader charge of BC_2N monolayer without and with Li adsorption. The C, B and N bader charege of Li adsorption BC_2N monolayer were selected near the Li atom.

C1	C2	B	N	Li
0.51	-0.48	1.57	-1.6	
0.53	-0.75	1.35	-1.44	0.75

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