Intercalation Mechanism of C_2N/Blue Phosphorene for Li-Ion Batteries: Ultrahigh Capacity, Fast Kinetics and Improved Compatibility with FSI/FEC Electrolytes

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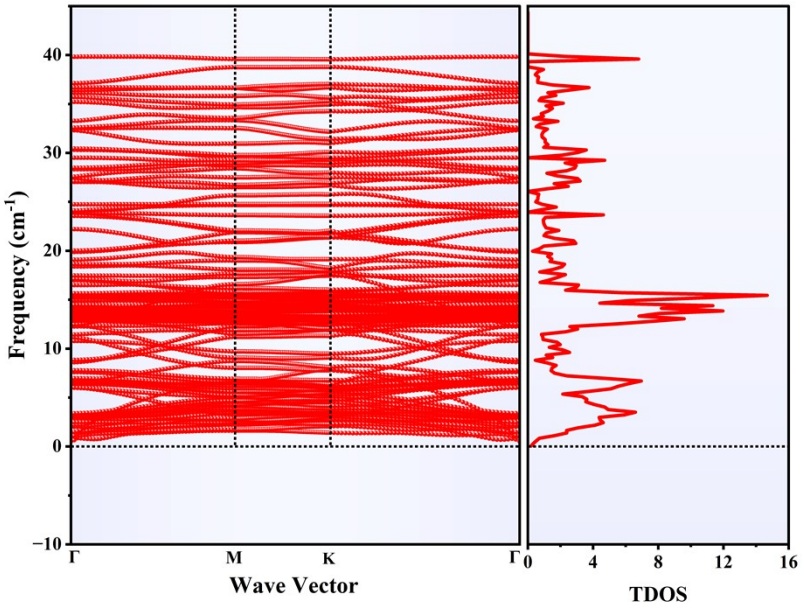

Figure S1. Computed phonon dispersion spectrum (Band&DOS) of the C_2N/BlueP heterostructure along the high-symmetry paths in the Brillouin zone.

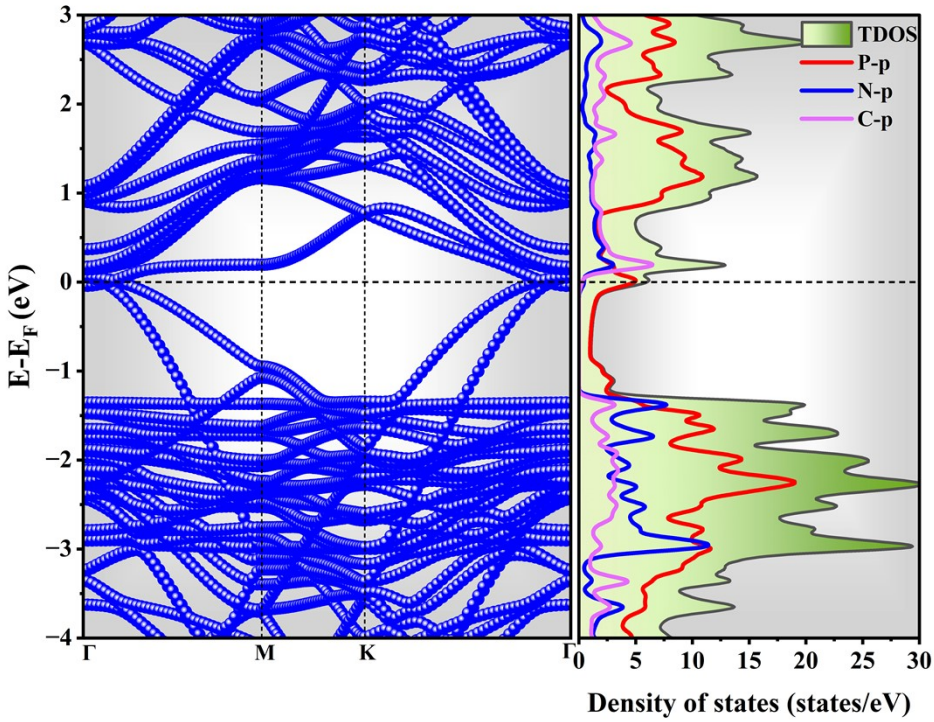

Figure S2. Band structure and total and partial electronic DOSs of the C_2N/BlueP heterostructure calculated using the GGA-PBE functional.

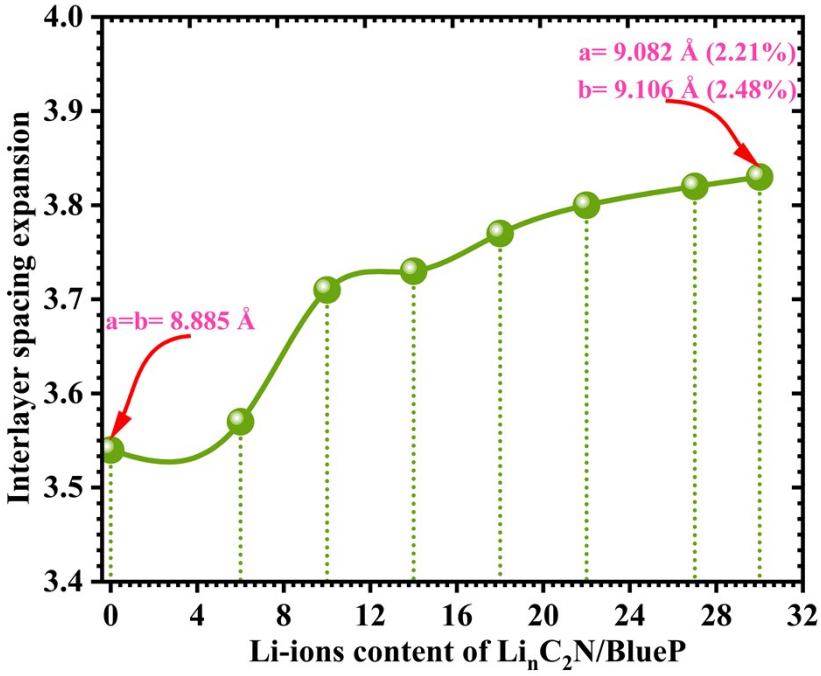

Figure S3. Interlayer spacing expansion during Li intercalation and the percentage of structural deformation in the in-plane lattice parameters.

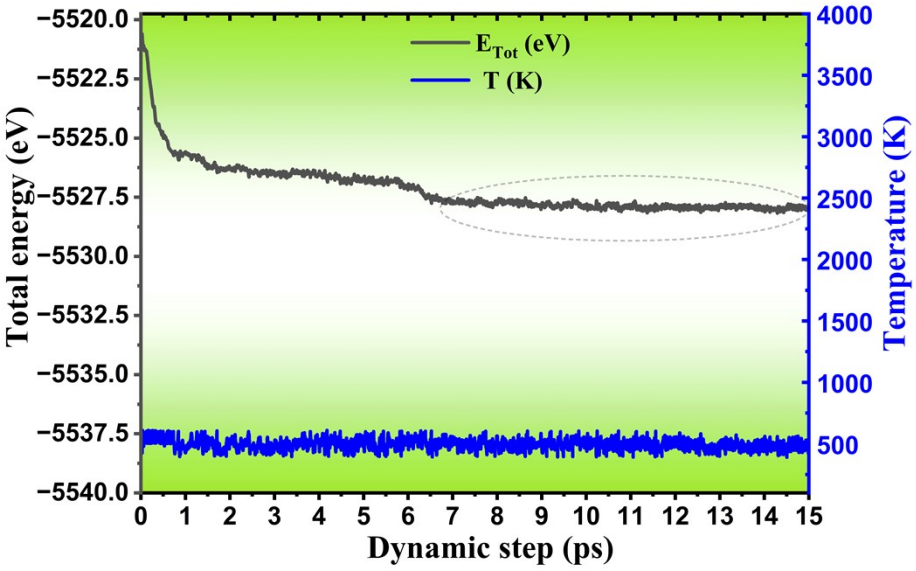

Figure S4. Temporal evolution of total energy and temperature for the fully lithiated C_2N/BlueP structure obtained from a 15 ps AIMD simulation at 500 K.

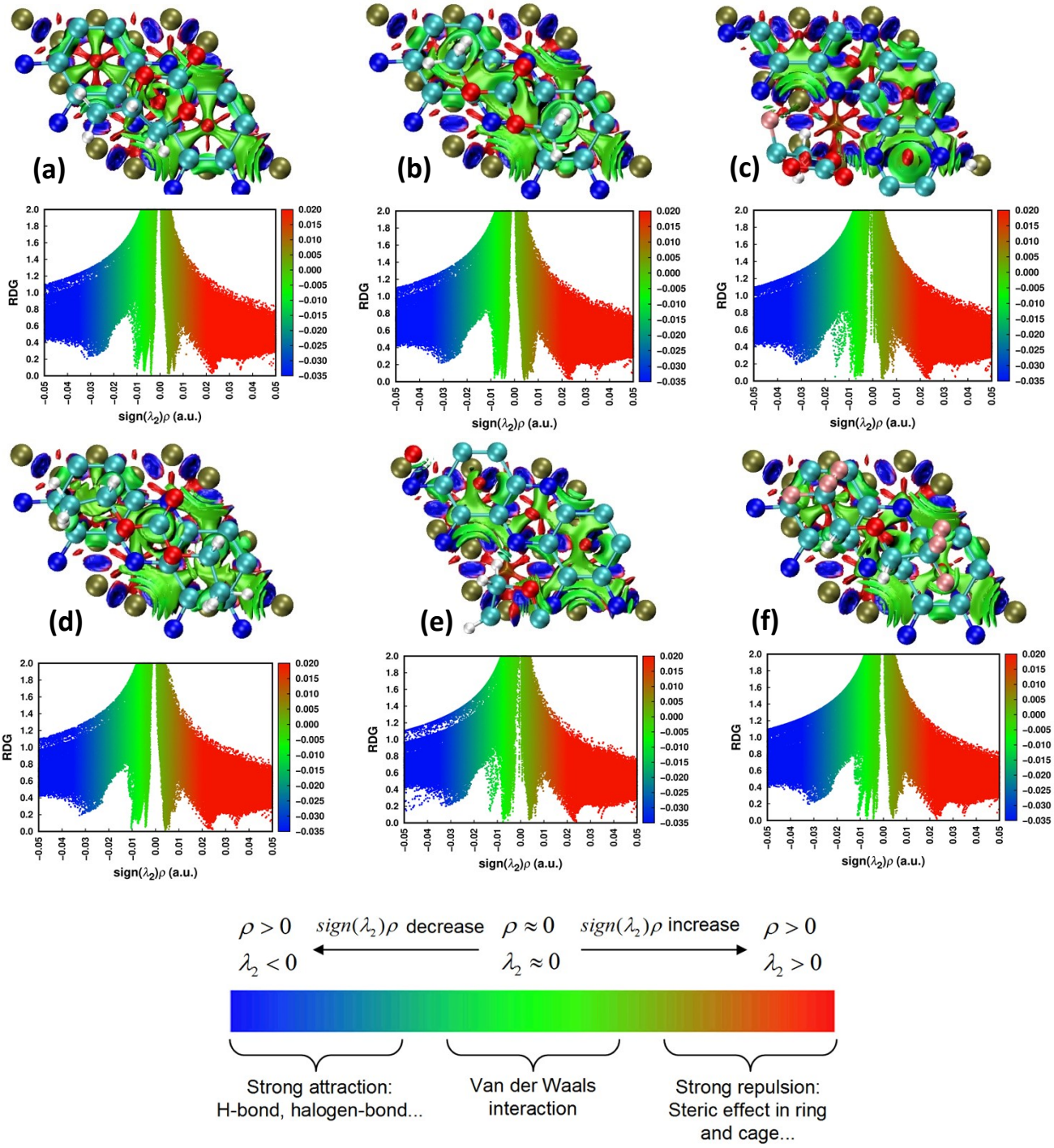

Figure S5. RDG isosurfaces and corresponding sign(λ_2)ρ plots for solvent adsorption on the anode: (a) BTFE, (b) DEC, (c) DMC, (d) EC, (e) FEC, and (f) PC solvent interactions with the anode.