SUPPORTING INFORMATION

Exploring the Potential of 2D Beryllonitrene as a Lithium-Ion Battery Anode: A Theoretical Study

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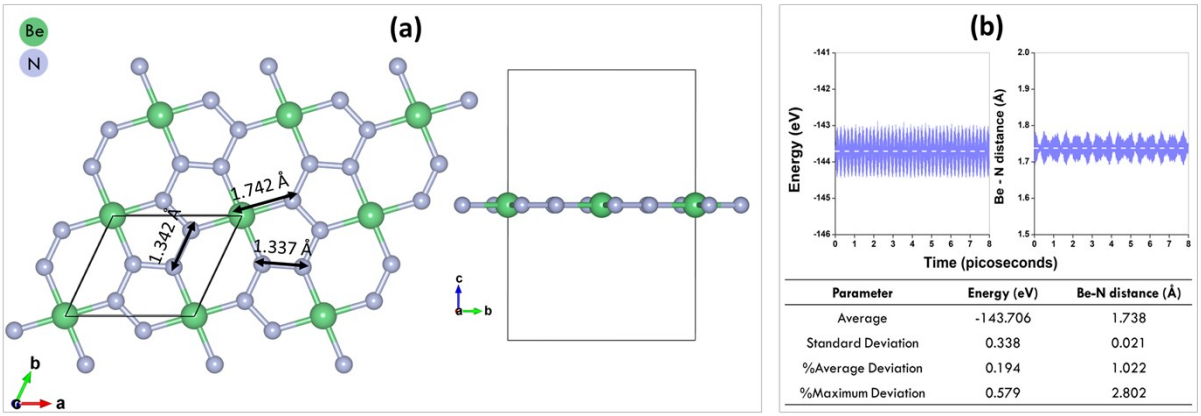

Parameter	Energy (eV)	Be-N distance (Å)
Average	-143.706	1.738
Standard Deviation	0.338	0.021
%Average Deviation	0.194	1.022
%Maximum Deviation	0.579	2.802

Figure S1: A 2 × 2 supercell of pristine BeN_4 (a) geometry optimized structure plot showing the bond distances (colour legend is inset to the top-left) in the top- and side-view; the unit cell is marked in black within and; (b) analysis of the ab initio molecular dynamics (AIMD) simulations of BeN_4 after 8 picoseconds at 300 K showing the energy (left panel) and Be-N bond length (right panel) fluctuations over time, with the average, standard, and percentage average and maximum fluctuations mentioned in the table (bottom panel).

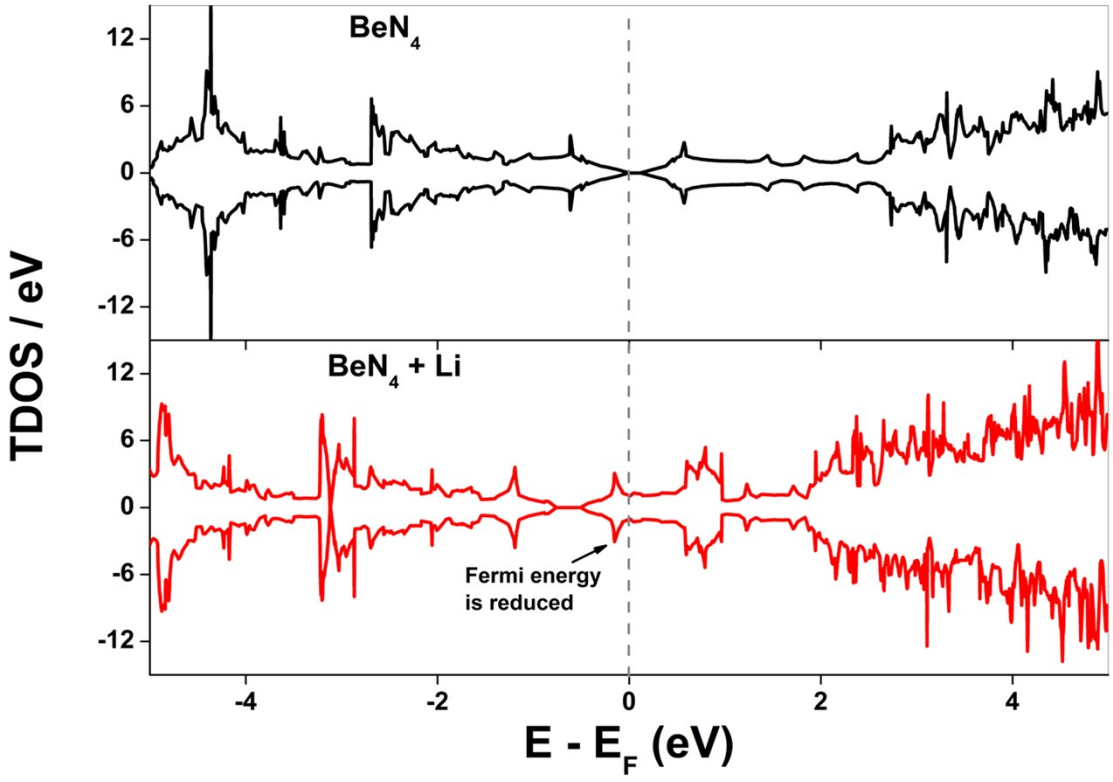

Figure S2: Electronic structure of BeN_4 and lithiated BeN_4 monolayers: Total density of states (TDOS) analysis of BeN_4 and BeN_4 + Li. The Fermi level is represented by a dashed line and set to 0 eV.

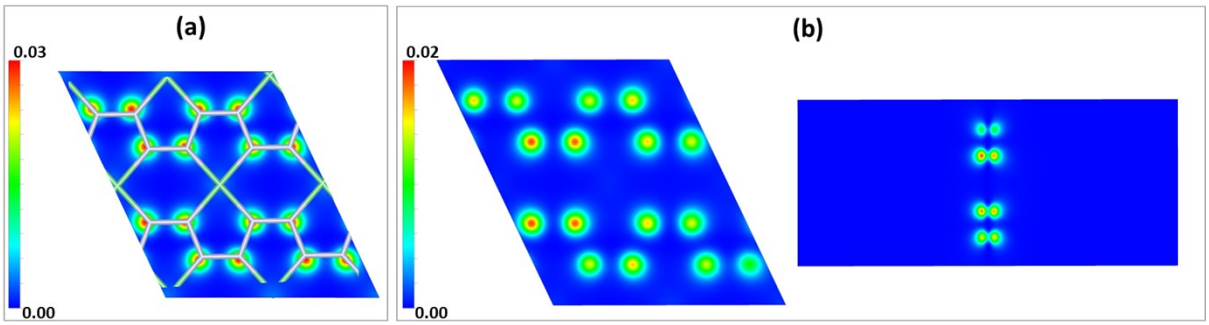

Figure S3: Orbital plot from the partial charge density distribution for (a) pristine BeN_4 and (b) BeN_4 + Li in the (left panel) molecular *xy* plane and (right panel) plane containing adsorbed Li and N atoms.

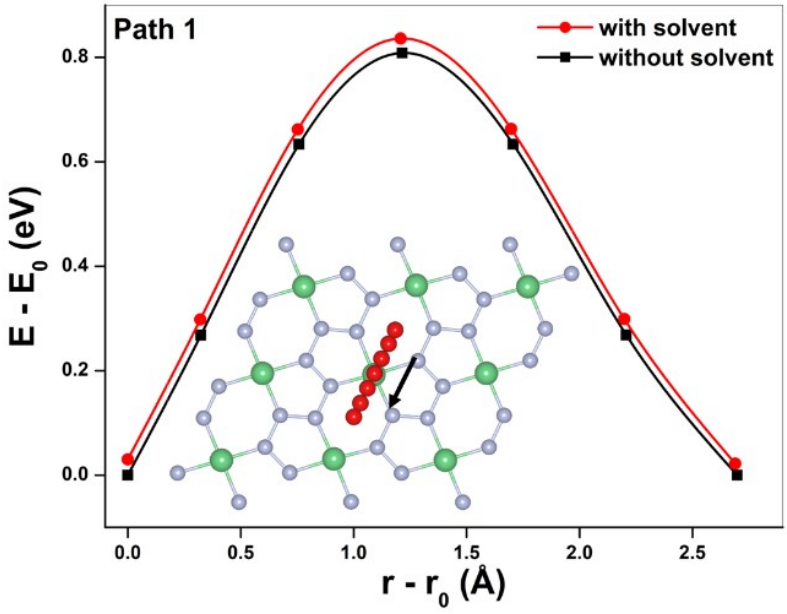

Figure S4: Diffusion energy barrier of Li^+ across BeN_4 computed with and without solvent effect (ethylene carbonate electrolyte) calculated using the Cl-NEB method.

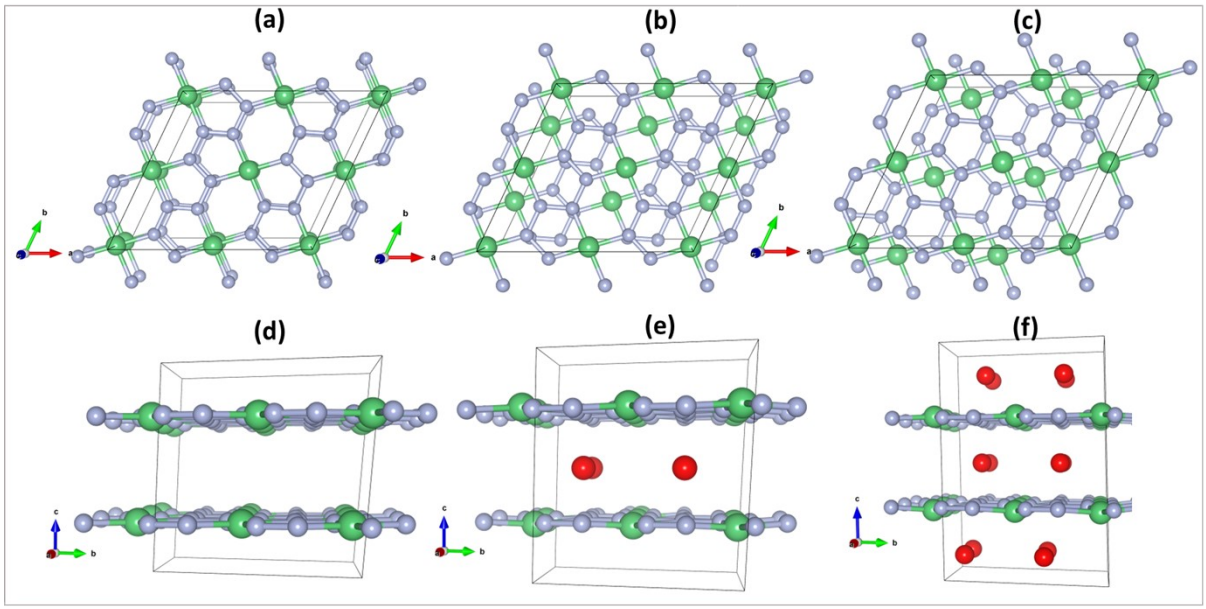

Figure S5: Geometry-optimized structure plots of (a–c) the three bilayer of 2D BeN_4 with (a) AA stacking, (b) AB(1) stacking, and (c) AB(2) stacking. The AB(2) bilayer was found to be the most table and Li^+ intercalation was studied for AB(2). (d) Side view of AB(2) bilayer from the *a* direction, (e) 4 Li^+ and (f) 12 Li^+ intercalated in AB(2).