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

Supplementary Information

Electronic, optical, and adsorption properties of Li doped hexagonal boron nitride: A GW approach

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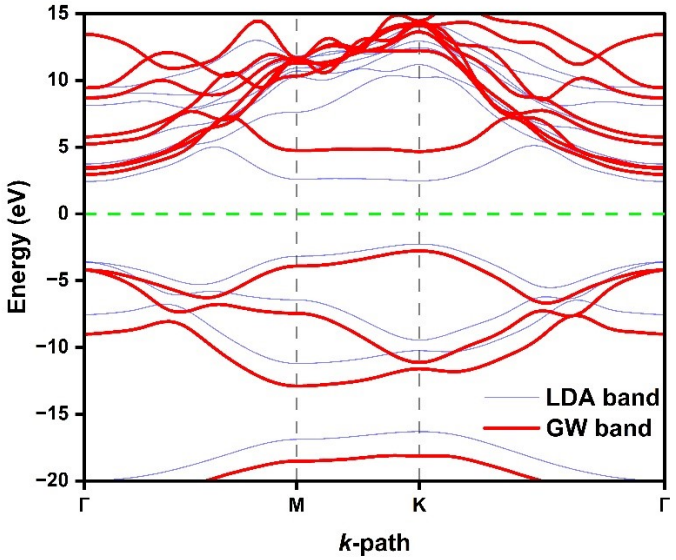

Figure S1: Band structure of pristine *h*-BN monolayer.

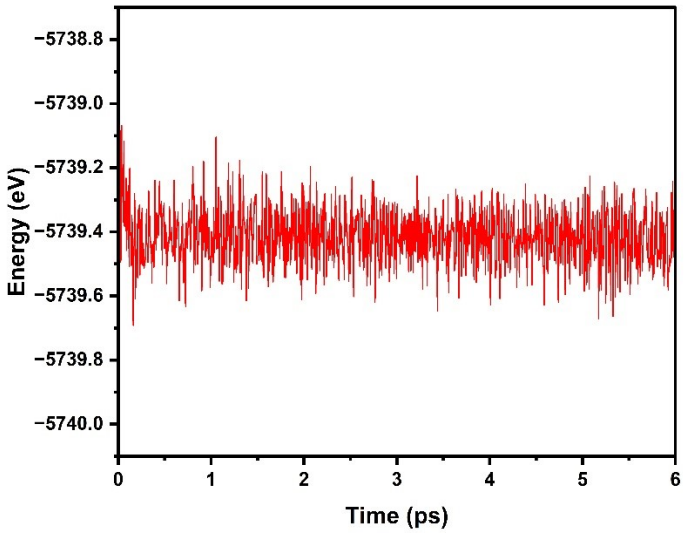

Figure S2: MD simulation at 300 K of *h*-BN^{Li} monolayer.

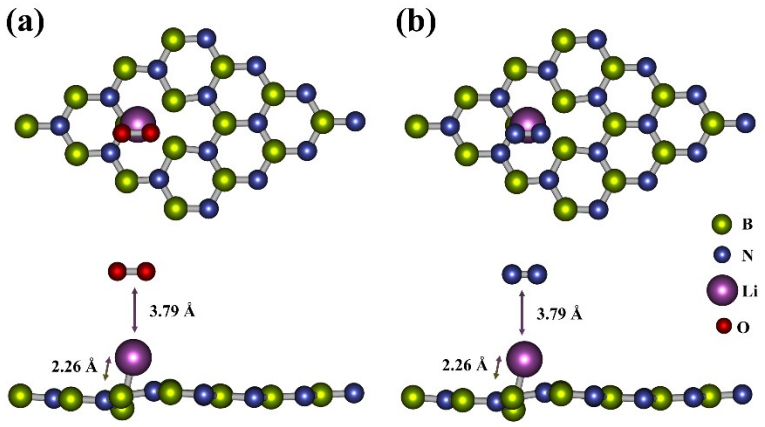

Figure S3: Optimised structures of (a) O_2 adsorbed *h*-BN^{Li}, and (b) N_2 adsorbed *h*-BN^{Li}.