

Supplementary Information

Porous BN for hydrogen generation and storage

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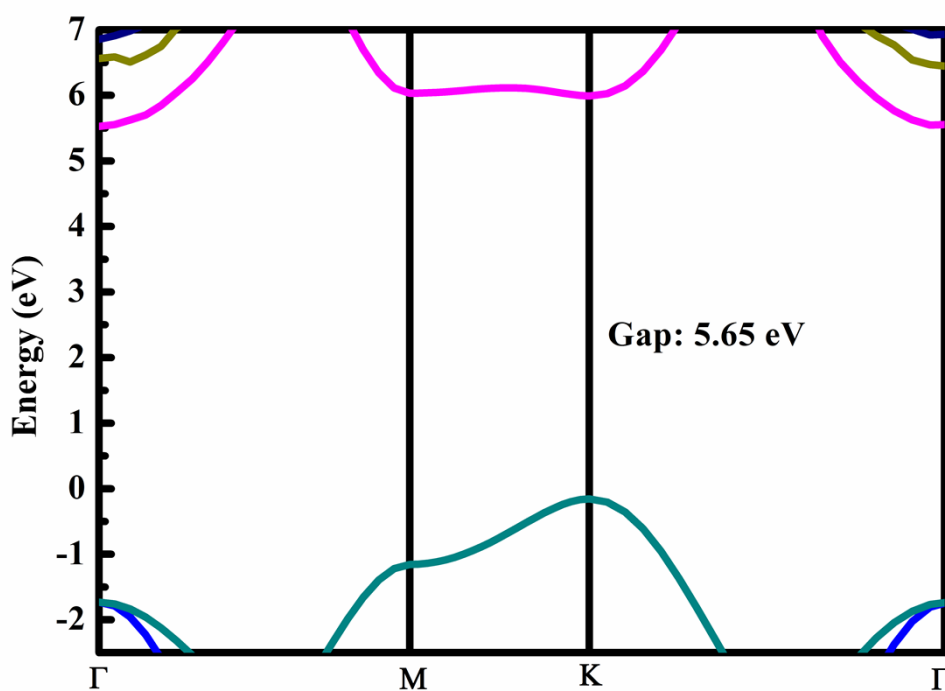


Fig. S1 Calculated band structure of ideal monolayer h-BN with the hybrid HSE06 functional.

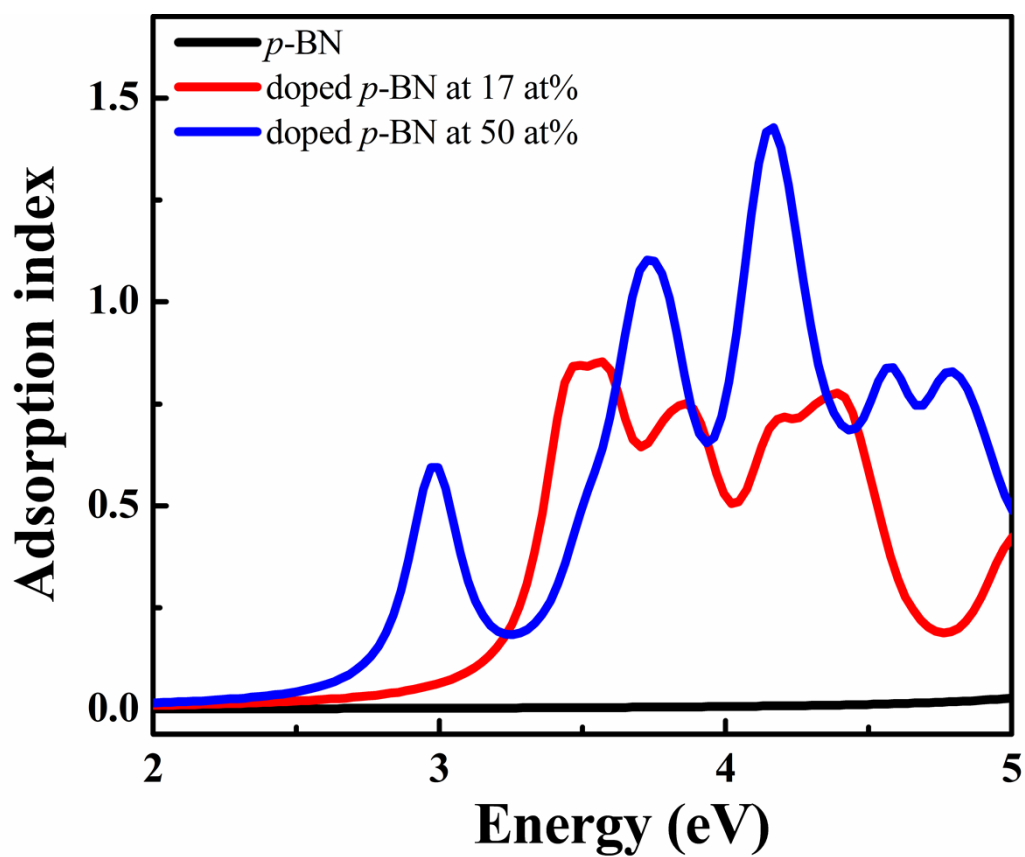


Fig. S2 Calculated optical absorption spectrum of the original and C-doped p-BN for the different constitute percentages with hybrid HSE06 functional.

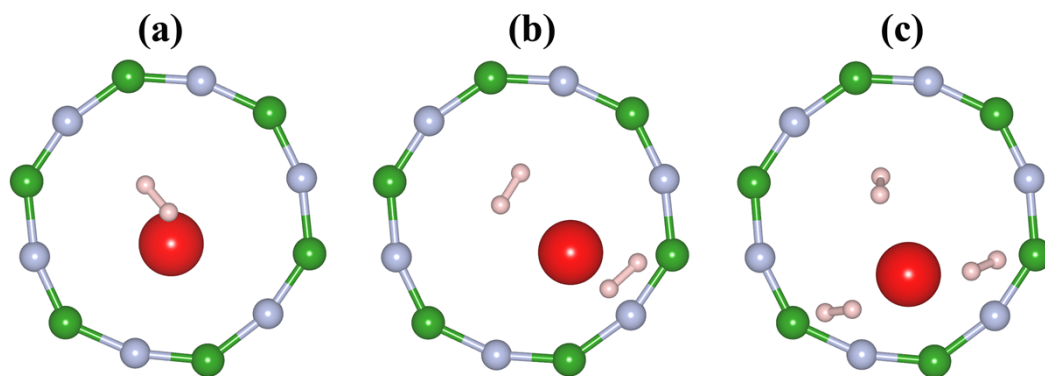


Fig. S3 The top view of atomic geometries of hydrogen on Li-decorated p-BN as the hydrogen capacity increases.

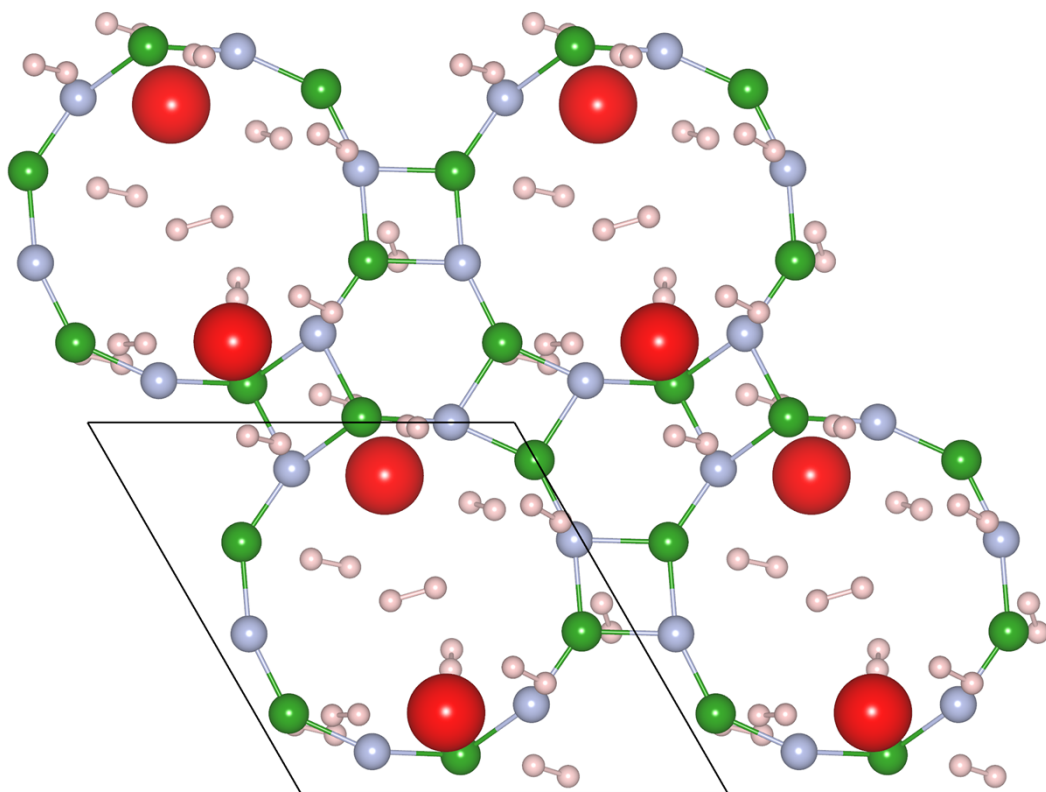


Fig. S4 the top view of optimized geometry with hydrogen adsorption on the two sides of Li-decorated p-BN.