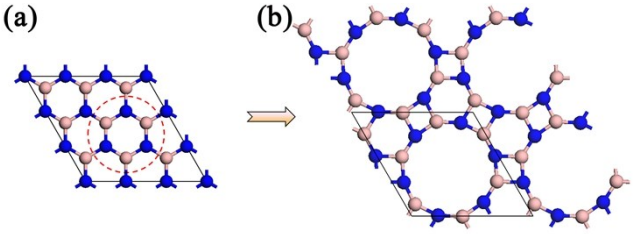

Fig. S1 The geometries of original (a) and optimized (b) porous BN (p-BN), respectively.

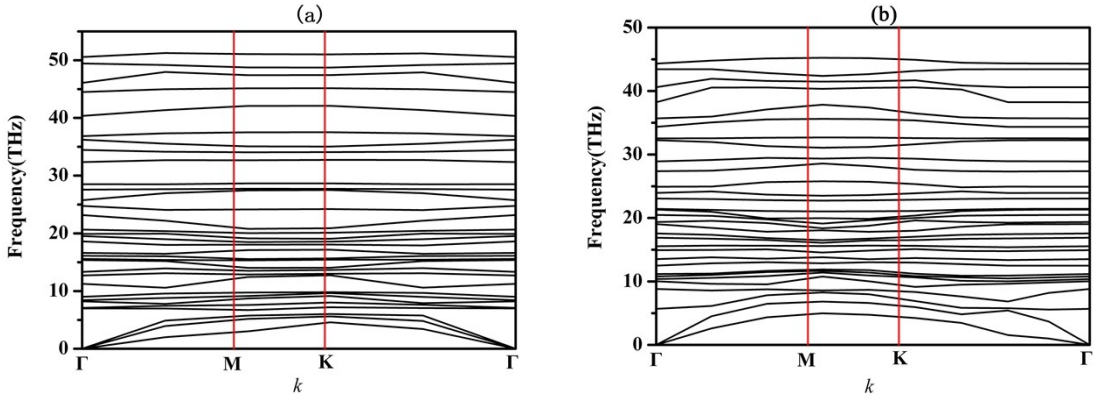

Fig. S2 The phonon dispersions of (a) p-BN with V_B defect and (b) p-BN with V_N defect

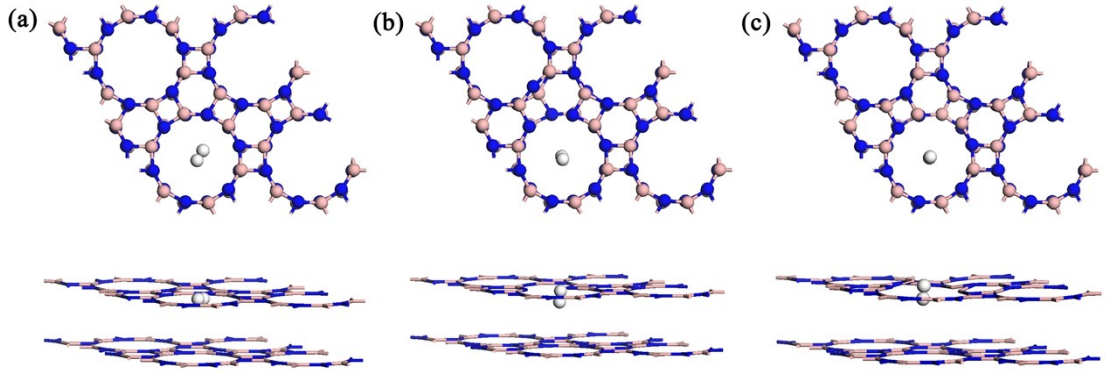

Fig. S3 Optimized geometric configurations of adsorbed H_2 on perfect p-BN (a), V_B defect (b), and V_N defect (c).

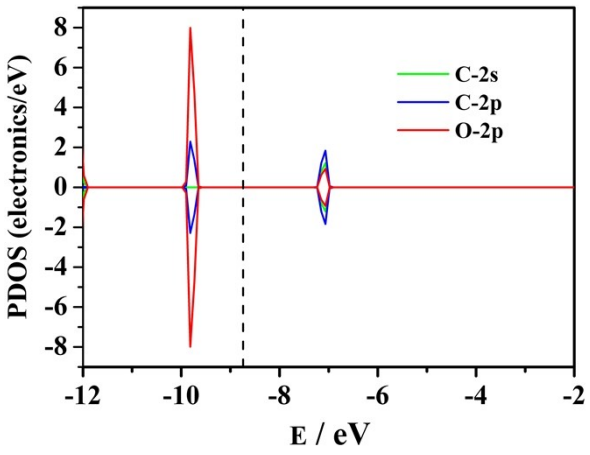

Fig. S4. Projected density of states (PDOS) for isolated CO molecule.

S1 computational details

The density-functional theory with dispersion（DFT-D）method were employed to improve the adsorption energies by the inclusion of long range interactions in the adsorption process. The computations (geometry optimizations, energy calculations) were performed using the PBE nonhybrid generalized gradient density functional coupled with long-range dispersion correction via Grimme's scheme[1] (PBE+D) as implemented in the DMol3 module in Materials Studio.[2,3] An all electron double-numeric atomic orbital augmented by polarization functions (DNP) has been chosen as basis set. This calculational level has been used to successfully study adsorptions, desorption, and the reaction mechanisms of some gases on boron-containing nanomaterials. [4, 5]

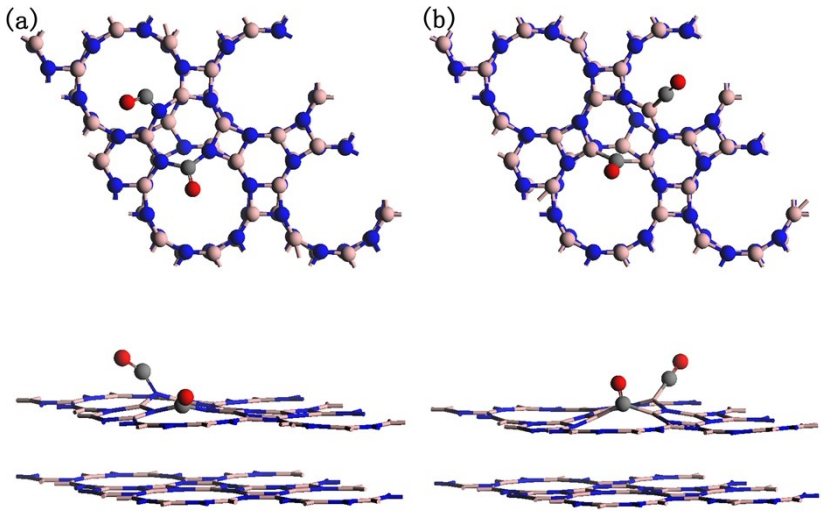

Fig. S5. Optimized geometric configurations of adsorbed two CO molecules on V_B defect(a), and V_N defect(b).

References

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