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

Theoretical study of the nitrogen reduction reaction catalyzed by B-doped MoO_2 six-membered ring

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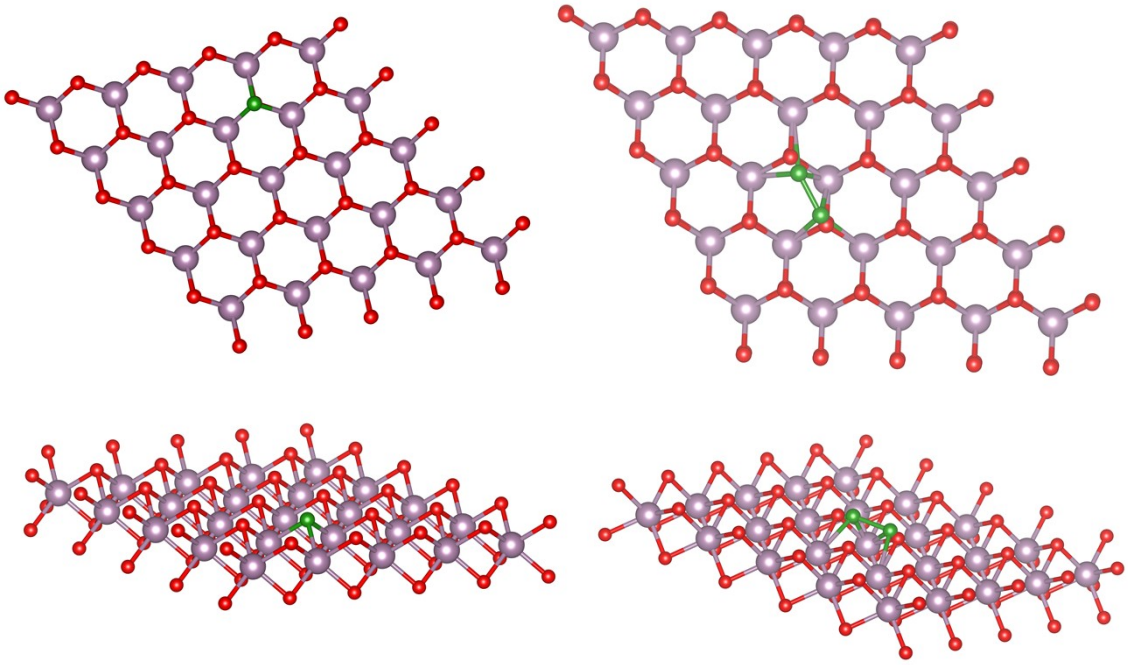

Figure S1. Double B monoatom doped MoO_2 configuration (B_2/MoO_2) (right) and B atom doped MoO_2 configuration (B/MoO_2) (left).

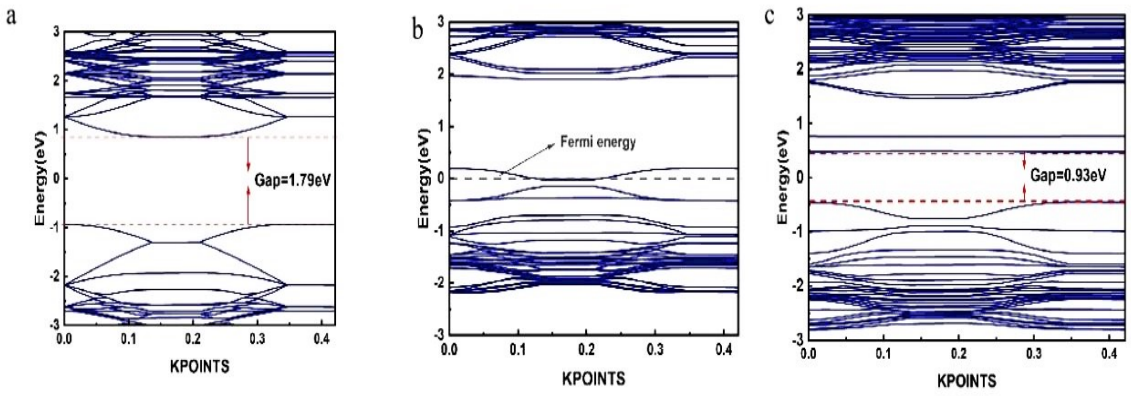

Figure S2. Energy band structure diagrams of a) MoO_2, b) B/MoO_2 and c) B_2/MoO_2.

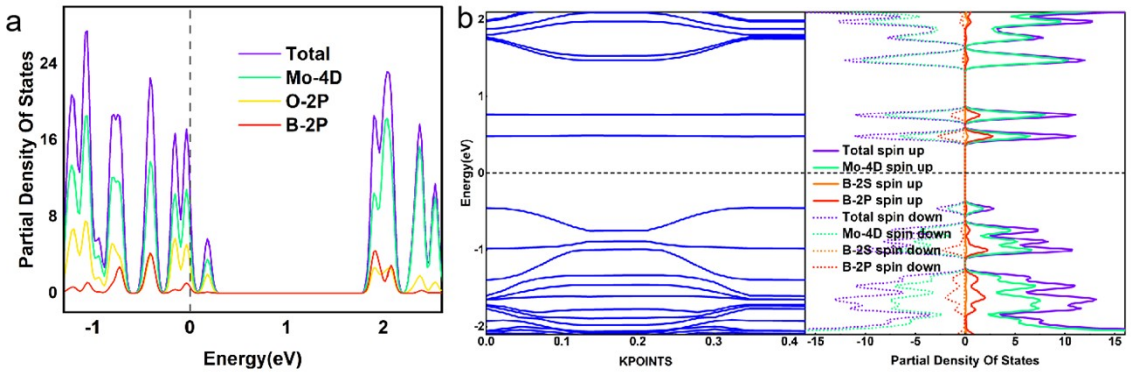

Figure S3. a) density of states plot of B/MoO_2; b) projected density of states plot of B_2/MoO_2.

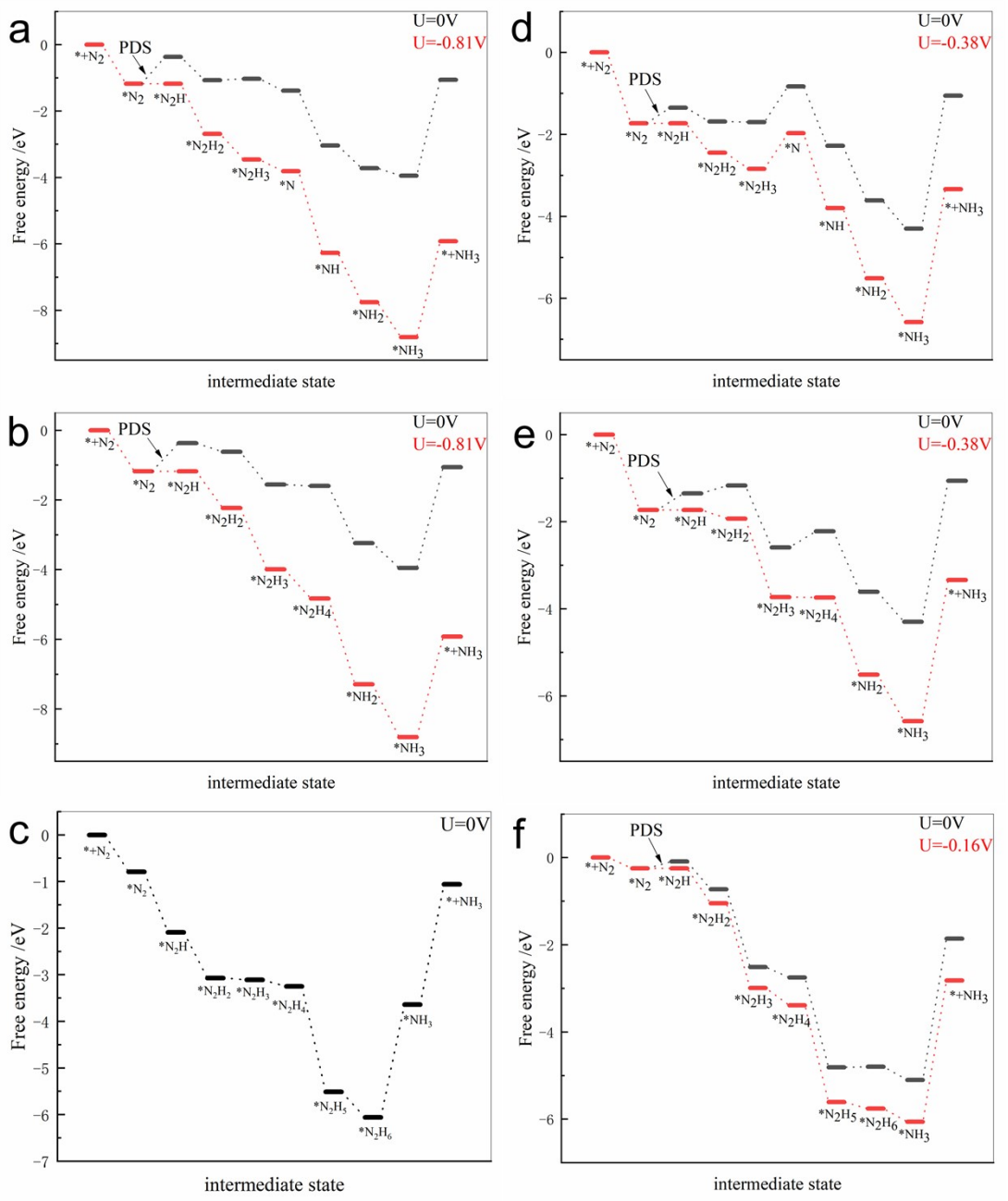

Figure S4. Free energy for the formation of various intermediates during the reduction of N_2 to ammonia in the enzymatic (a), distal (b), and alternating (c) pathways on B_2/MoO_2, and in the enzymatic (d), distal (e), and alternating (f) pathways on B/MoO_2.

Table S1 bader charge analysis for different adsorption configurations

adsorption configurations	sub	B2	N_2
N_2-B_2 (side)	-0.04 e	0.01 e	0.03 e
N_2-B_2 (terminal)	0.16 e	0.09 e	-0.25 e
N_2-B (side)	0.10 e	0.08 e	-0.19 e
N_2-B (terminal)	0.12 e	0.11 e	-0.22 e