Supporting Information for "Theoretical screening of efficient single-atom catalysts for nitrogen fixation based on defective BN monolayer"

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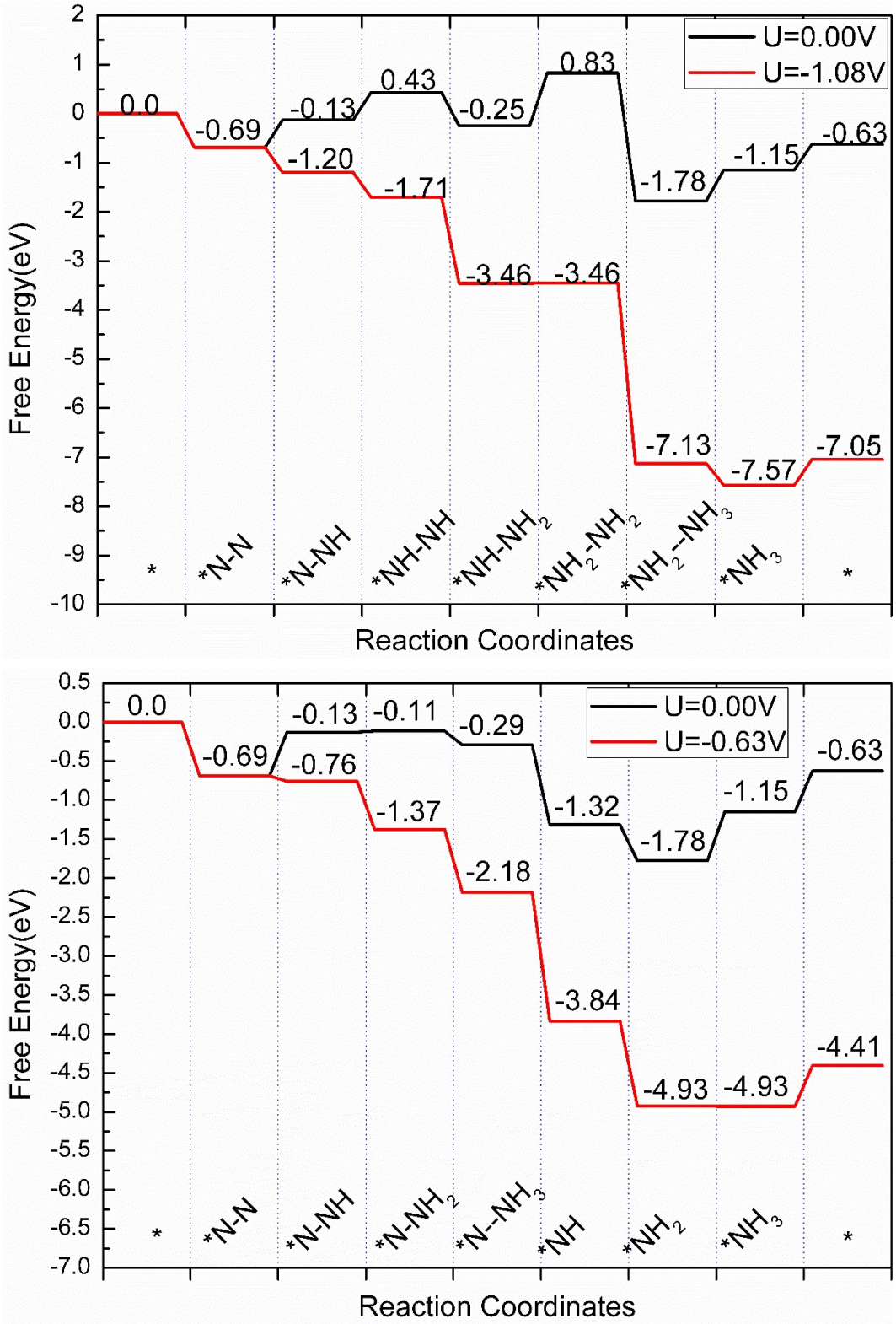

Fig. S1 The calculated free energy diagrams of NRR on the plane of Tc@BN through alternating (a) and distal (b) pathway.

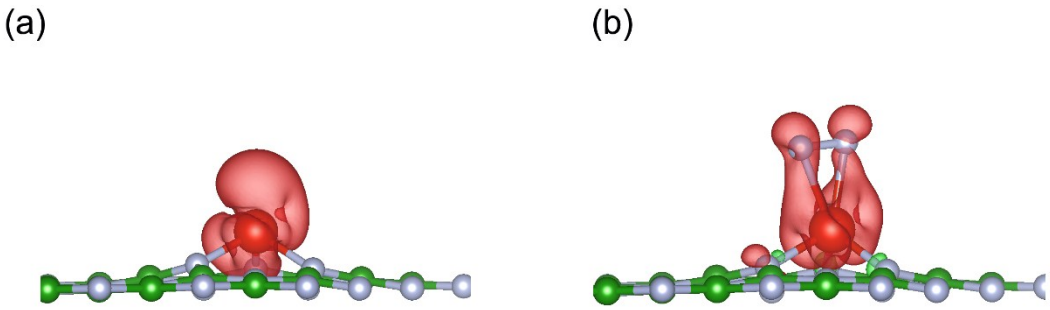

Fig. S2. The Spin density of V@BN before (a) and after (b) N2 adsorption.

Table S1. The Bader charge of V atom, three-coordinated N atoms (N1, N2, and N3) in h-BN and N_2 molecular in V@BN and N_2 adsorbed V@BN, respectively.

	V	N1	N2	N3	N_2
V@BN	-1.41	1.88	1.89	1.88	
N2*V@BN	-1.75	1.85	1.88	1.85	0.51