Electronic Supplementary Information

Improved Nitrogen Reduction Activity of $NbSe_2$ Tuned by Edge Chirality

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Table S1 H adsorption energy on $NbSe_2$ edges.

$NbSe_2$ edge model	H adsorption energy (eV)
Zigzag	–0.16
Zigzag with one Se vacancy	–1.79
Armchair	0.28
Armchair with one Se vacancy	0.29

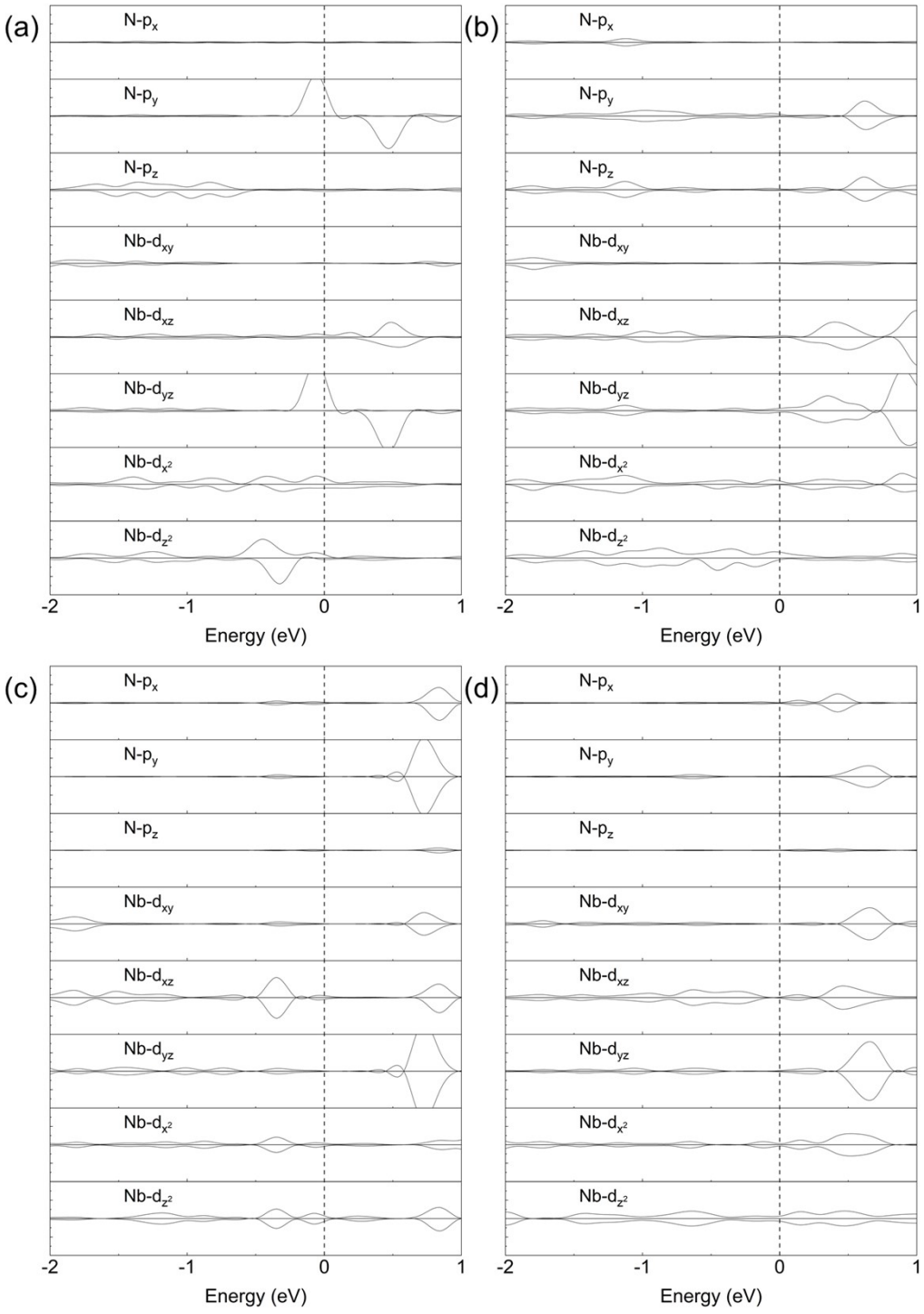

Figure S1. Density of states projected on (PDOS) N 2p states and Nb 4d states on (a) zigzag edge and (b) zigzag edge with one Se vacancy via side-on pattern, (c) armchair edge and (d) armchair edge of $NbSe_2$ via end-on pattern, respectively.

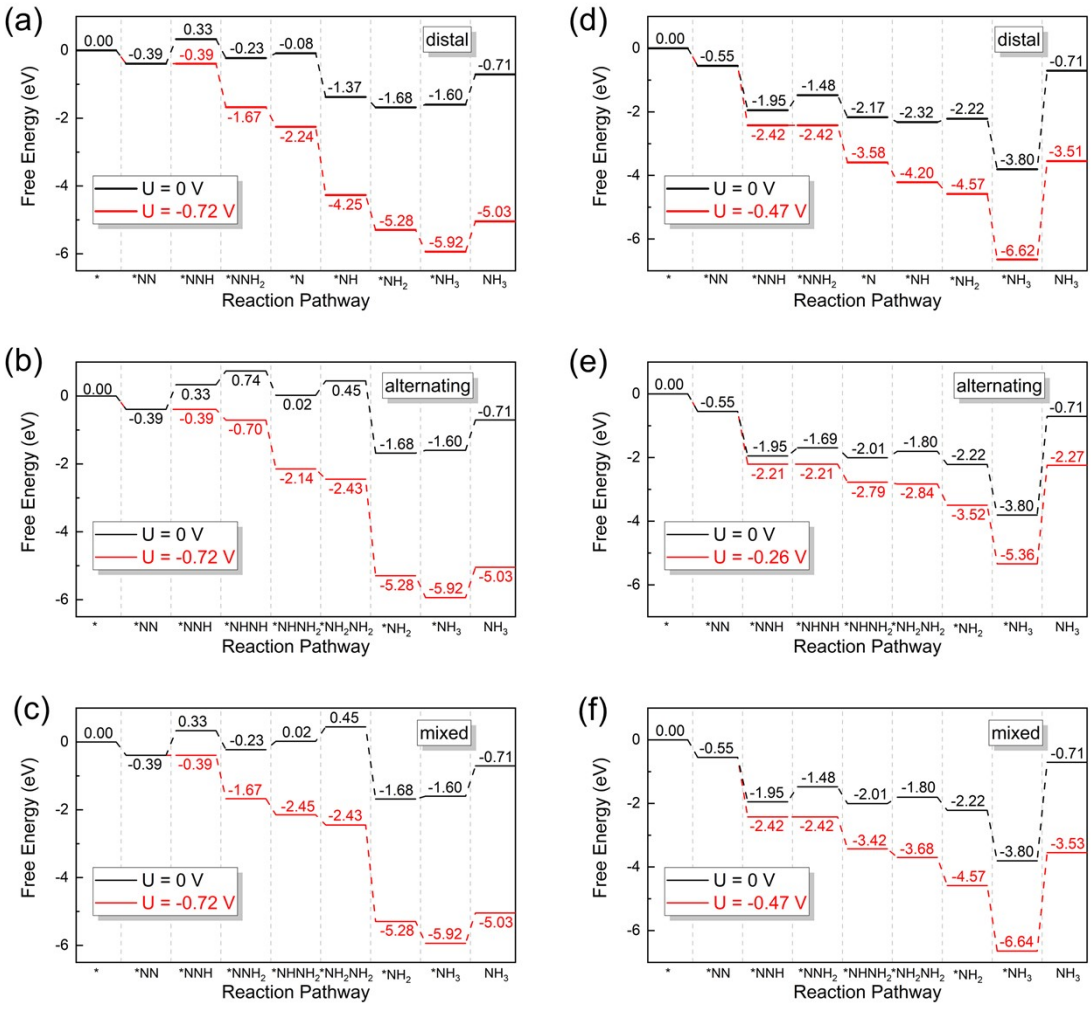

Figure S2. Gibbs free energy diagrams of distal, alternating and mixed pathway on pristine zigzag edge (a) (b) (c), zigzag edge with a Se vacancy (d) (e) (f).

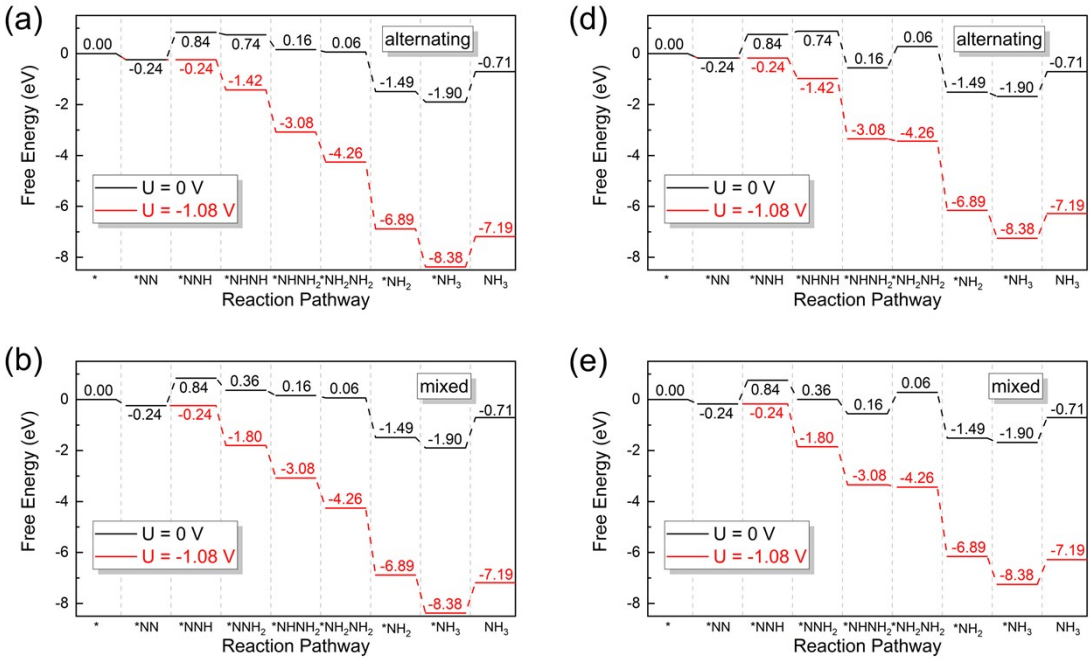

Figure S3. Gibbs free energy diagrams of alternating and mixed pathway on pristine armchair edge (a) (b), armchair edge with a Se vacancy (c) (d).