Supporting Information

for

Si@SbN: A promising solar photocatalyst for the reduction of NO

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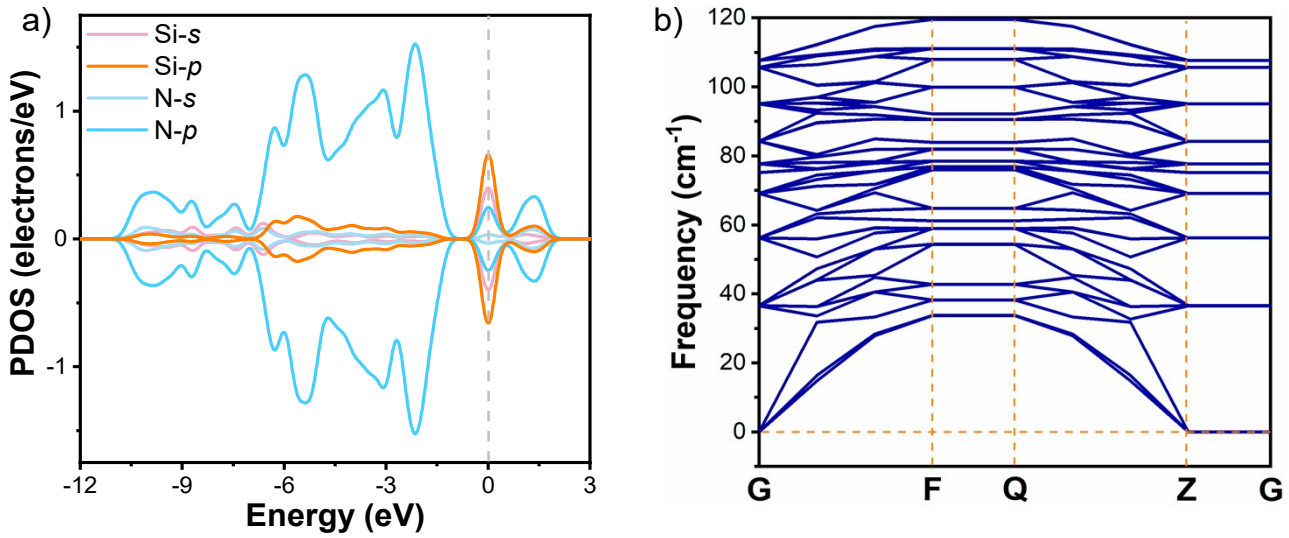

Figure S1. (a) Partial density of states (PDOS) of Si@SbN, including the N-*s*, Si-*s*, N-*p* and Si-*p* orbitals. (b) Phonon dispersion curve of geometrically optimized Si@SbN.

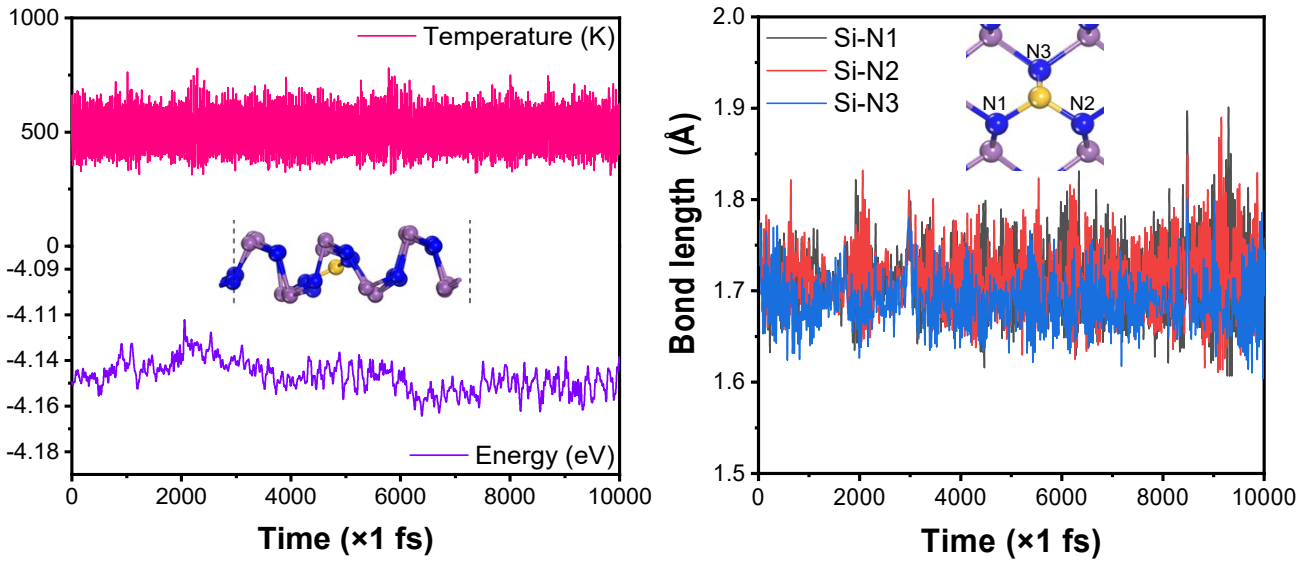

Figure S2. Variations of temperature, energy, and Si-N bond length fluctuations versus the AIMD simulation time for Si@SbN. The simulation is run under 500 K for 10 ps with a time step of 1 fs.

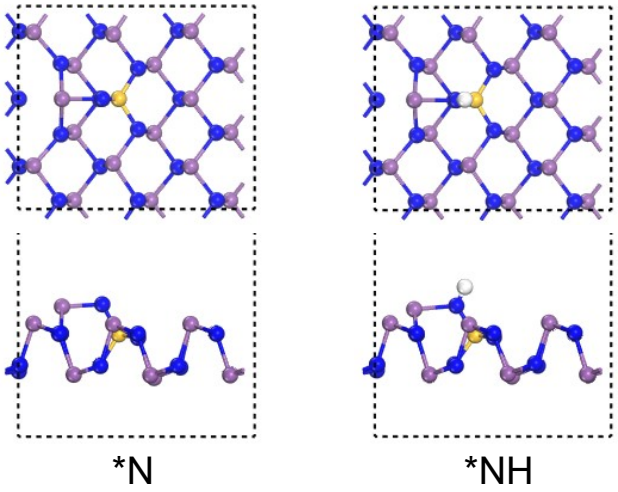

Figure S3. Optimized atomic configuration of *N and *NH.

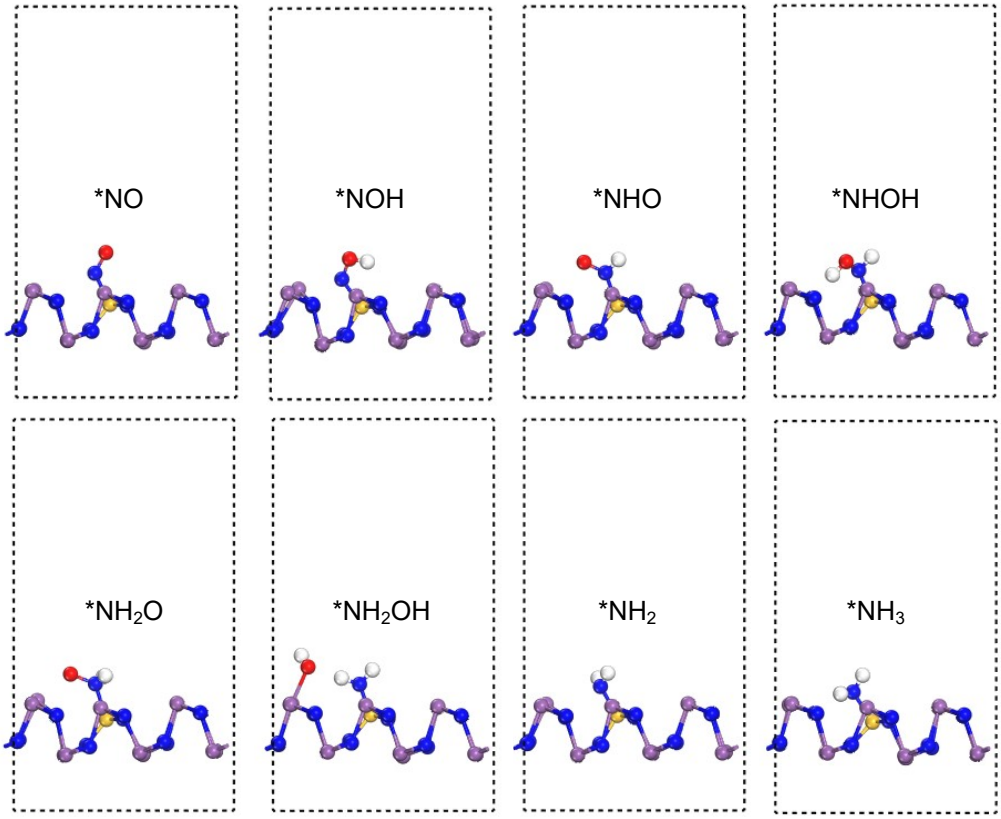

Figure S4. Optimized geometric of various intermediates along the different reaction pathways of NORR preceeded on Si@SbN.

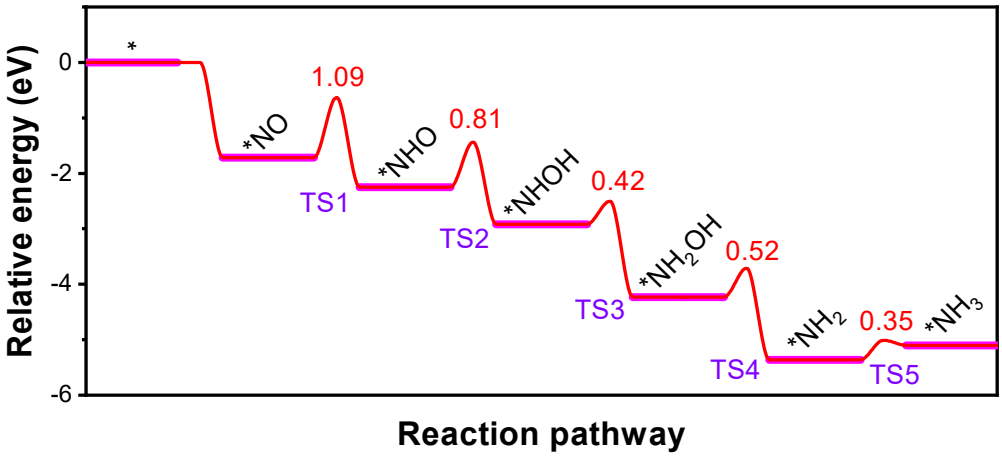

Figure S5. Energy barriers of each NORR step.

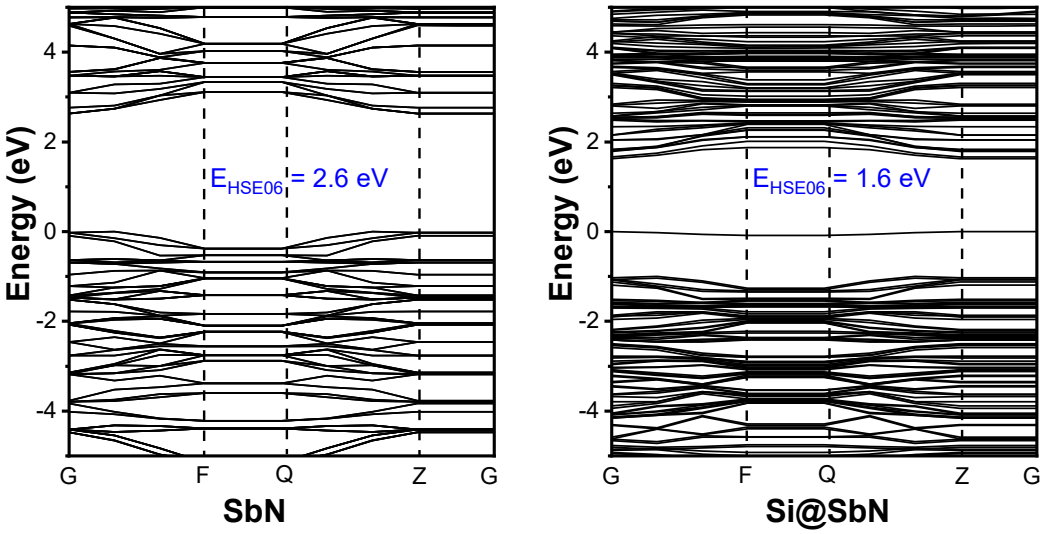

Figure S6. Band structures of (a) SbN and (b) Si@SbN.

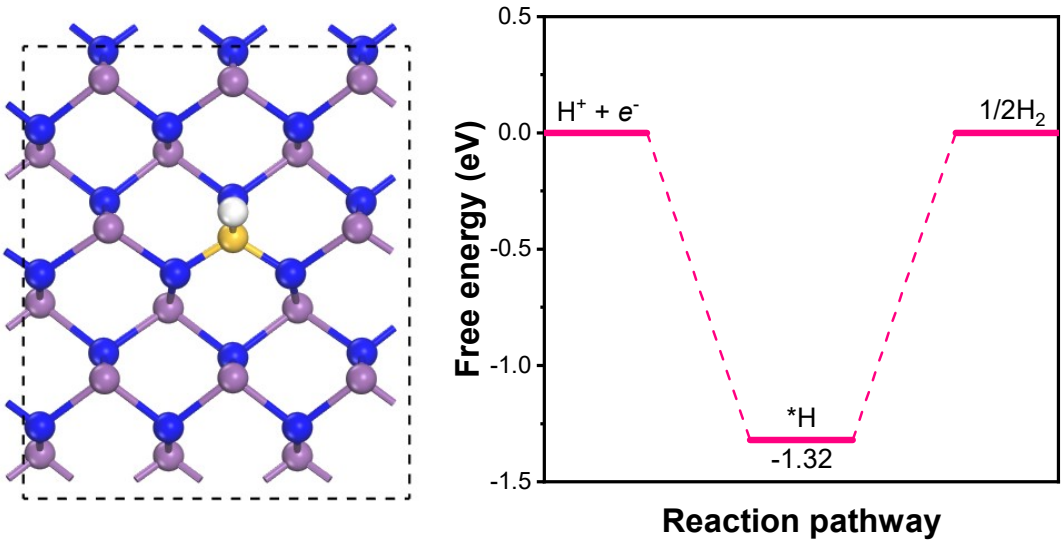

Figure S7. Optimized structure of *H adsorbed on Si@SbN and the corresponding free energy diagram of HER.

Table S1. Test of supercell size and doping concentration.

Supercell size	2 × 2 × 1	3 × 3 × 1	4 × 4 × 1
E_{ads}(*NO) (eV)	-1.89	-1.80	-1.78
Doping concentration	25.00%	11.11%	6.25%

Table S2. Formation energy (E_f, eV) of Si@SbN.

$E_{catalyst}$	E_{pure}	E_{Si}	E_{Sb}	E_f
-99817.82	-95774.67	-7874.95	-3833.42	-1.62

*****Formation energy (E_f), $E_f = E_{catalyst} - E_{pure} - E_{Si} + E_{Sb}$ where $E_{catalyst}$, E_{pure}, E_{Si} and E_{Sb} represent the DFT energy of Si@SbN catalyst, the DFT energy of pure SbN, the DFT energy of a Si atom in corresponding bulk, and the DFT energy of a Sb atom in corresponding bulk, respectively.