Electronic Supplementary Material (ESI) for Materials Advances.

Supporting Information for "Design for non-transition metal doped nanoribbons catalysis to achieve efficient nitrogen fixation"

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Table S1. Limiting Potential and corresponding Potential determining step for 16 SAC@GNR systems.

SAC	Lowest Limiting Potential(eV)	Potential determining step	Optimal Hydrogenation Mechanism
Be	-0.59	$*N_2 \rightarrow *NNH$	alternating
B	-1.11	$*NH_2 \rightarrow *NH_3$	alternating
C	-0.89	$*NH_2 \rightarrow *NH_3$	distal/alternating
N	-1.18	$*N_2 \rightarrow *NNH$	distal
Mg	-1.19	$*N_2 \rightarrow *NNH$	alternating
Al	-1.04	$*NH_2 \rightarrow *NH_3$	alternating
Si	-0.45	$*N_2 \rightarrow *NNH$	alternating
P	-1.01	$*N_2 \rightarrow *NNH$	alternating
Ca	-0.91	$*N_2 \rightarrow *NNH$	alternating
Ga	-0.67	$*NH_2 \rightarrow *NH_3$	alternating
Ge	-1.54	$*N_2 \rightarrow *NNH$	distal/alternating
As	-1.13	$*N_2 \rightarrow *NNH$	distal/alternating
Sr	-1.11	$*N_2 \rightarrow *NNH$	alternating
In	-0.97	$*N_2 \rightarrow *NNH$	alternating
Sn	-1.69	$*N_2 \rightarrow *NNH$	alternating
Sb	-1.01	$*N_2 \rightarrow *NNH$	alternating

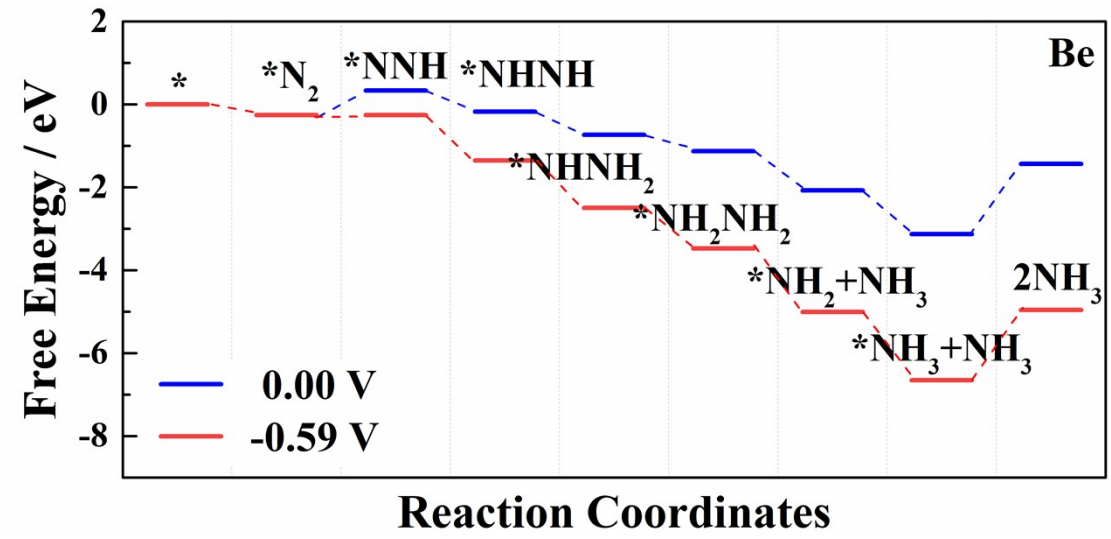
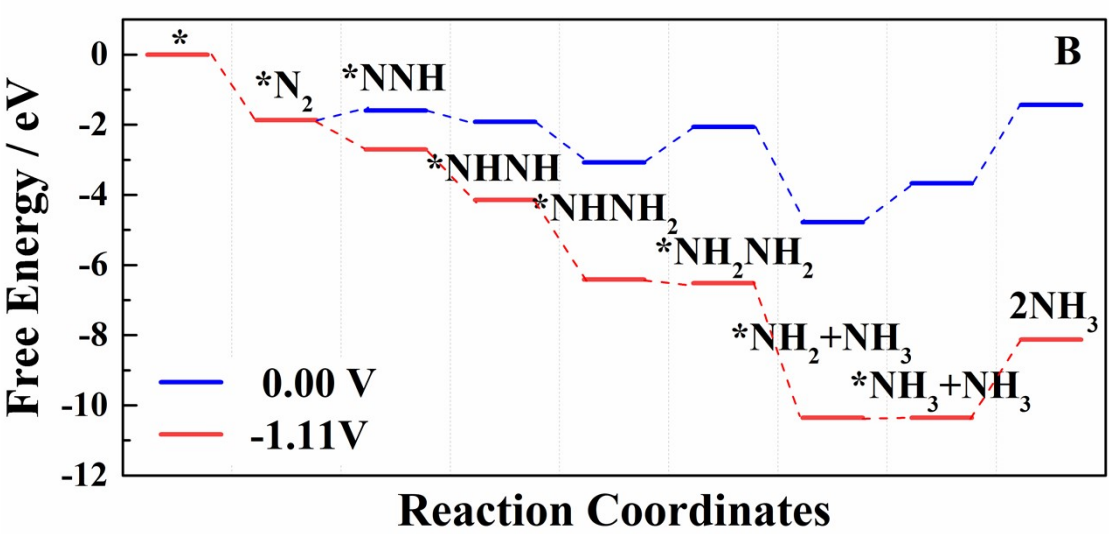


Figure S1. Free energy evolution process for Be@GNR system.



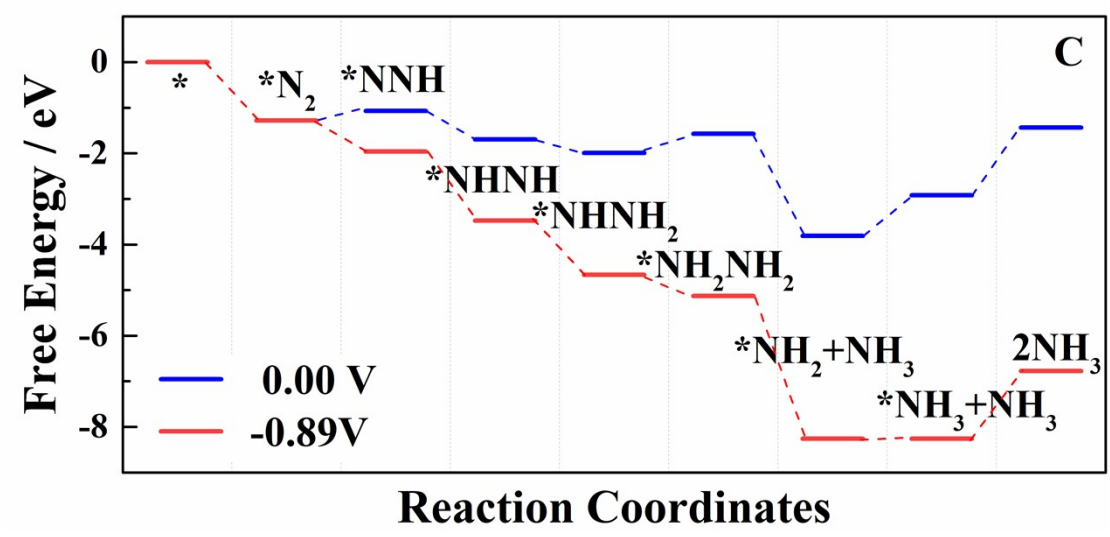


Figure S2. Free energy evolution process for B@GNR system.

Figure S3. Free energy evolution process for C@GNR system.

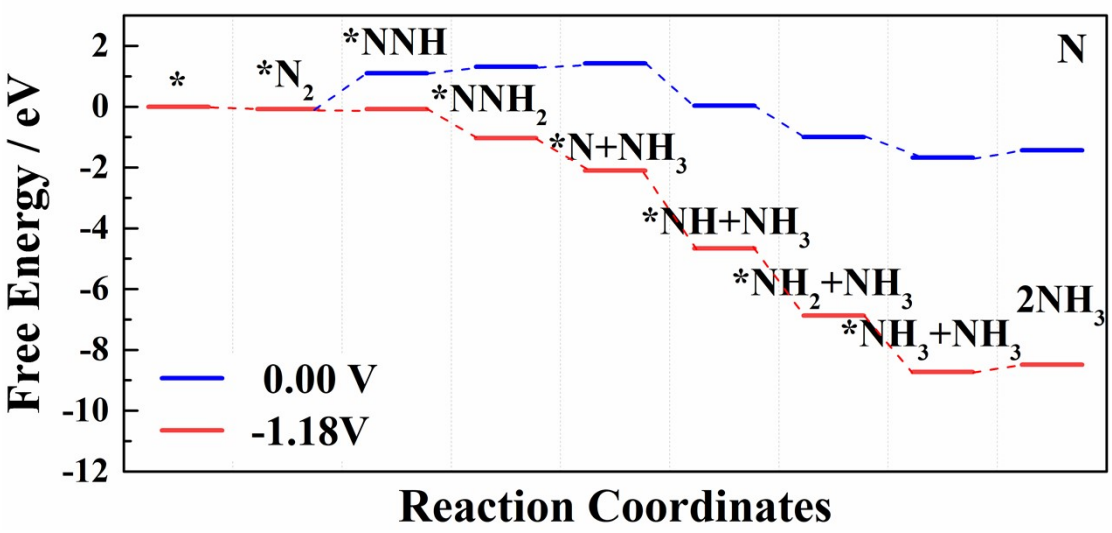


Figure S4. Free energy evolution process for N@GNR system.

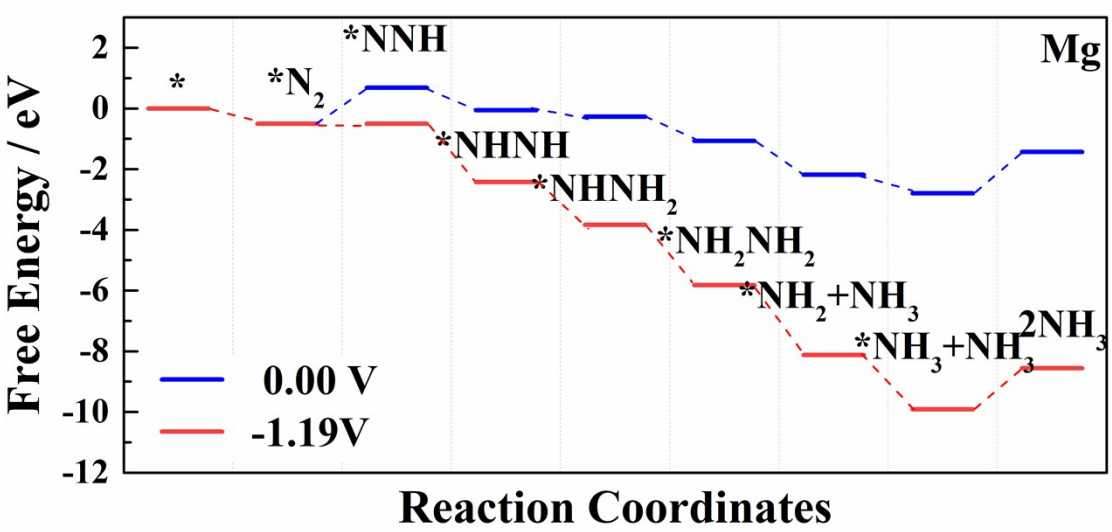


Figure S5. Free energy evolution process for Mg@GNR system.

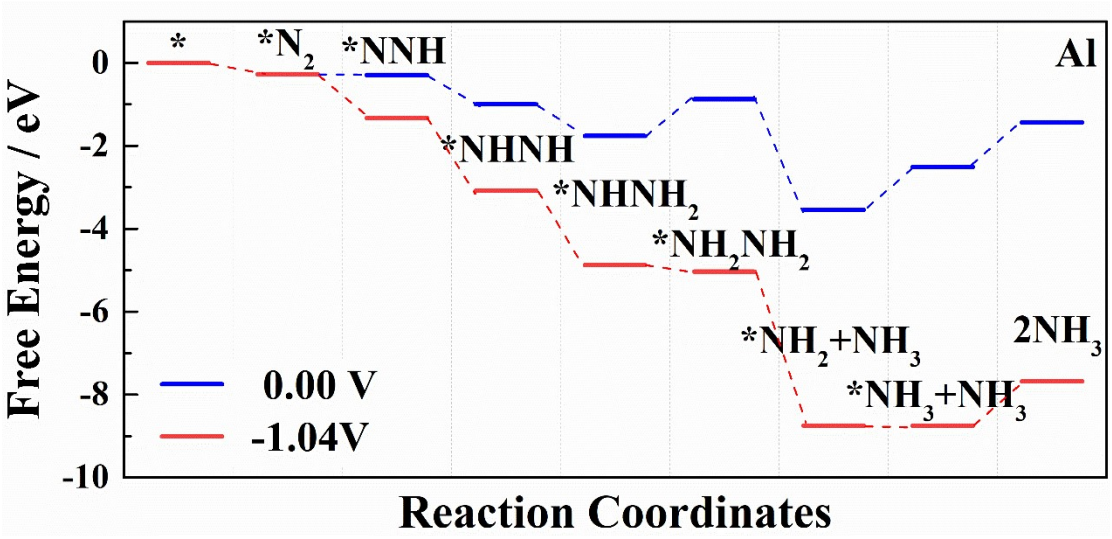


Figure S6. Free energy evolution process for Al@GNR system.

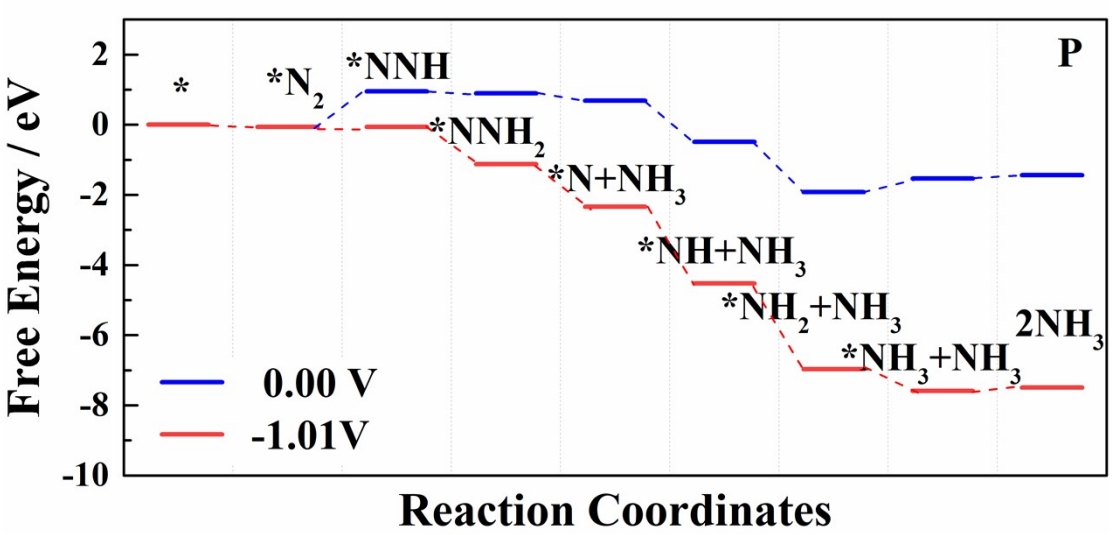


Figure S7. Free energy evolution process for P@GNR system.

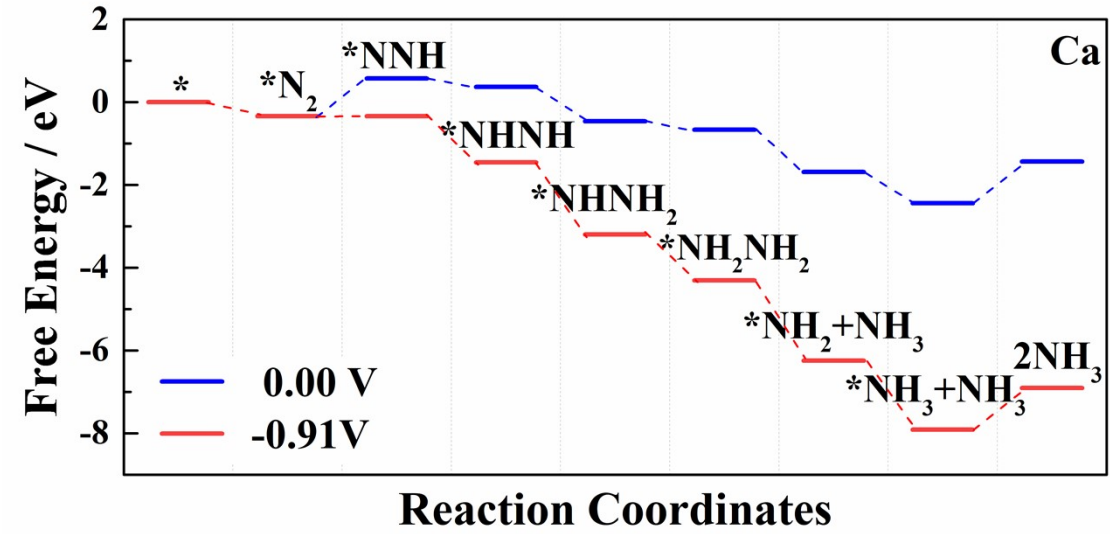


Figure S8. Free energy evolution process for Ca@GNR system.

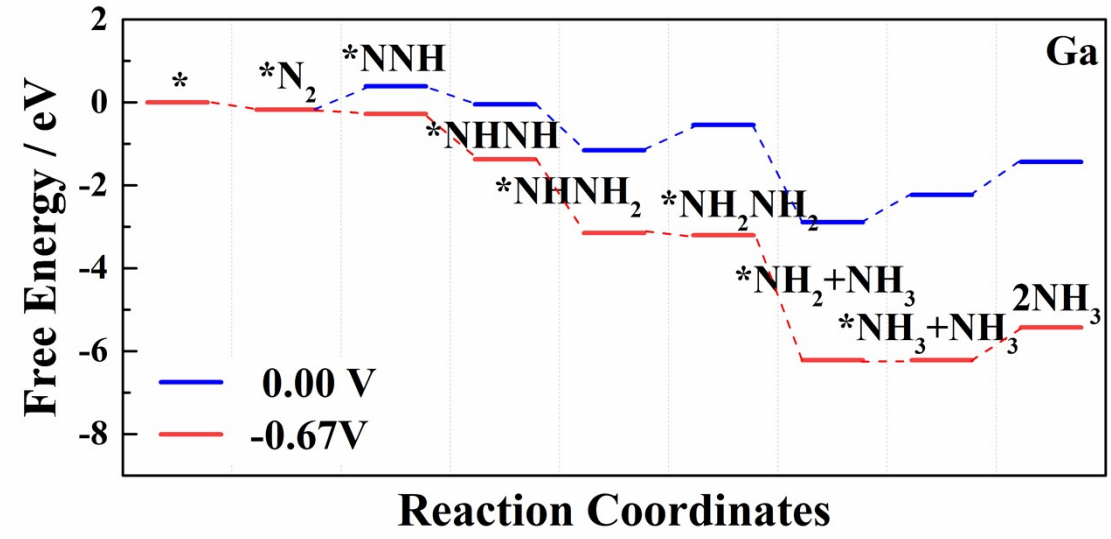


Figure S9. Free energy evolution process for Ga@GNR system.

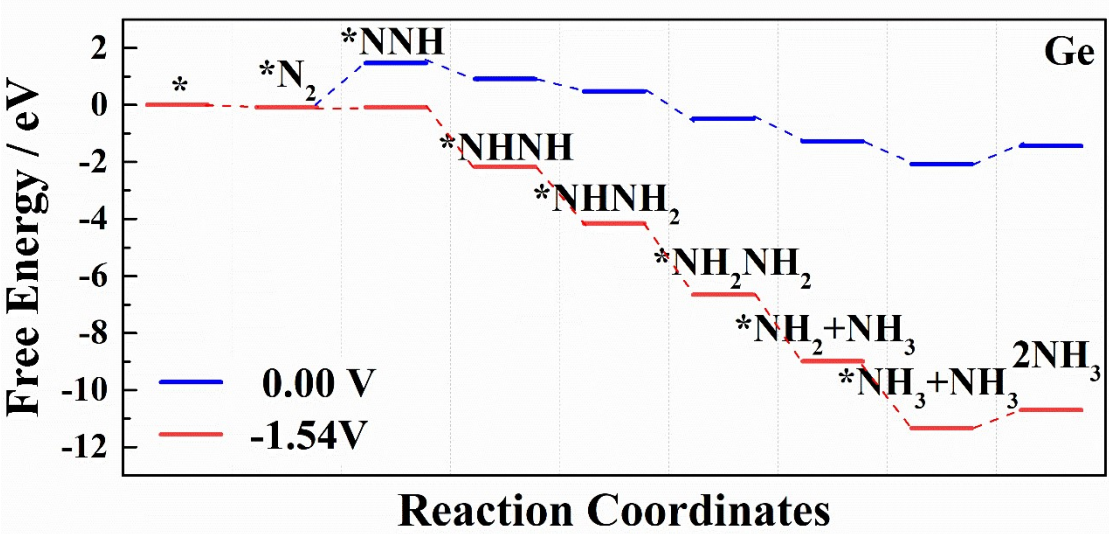


Figure S10. Free energy evolution process for Ge@GNR system.

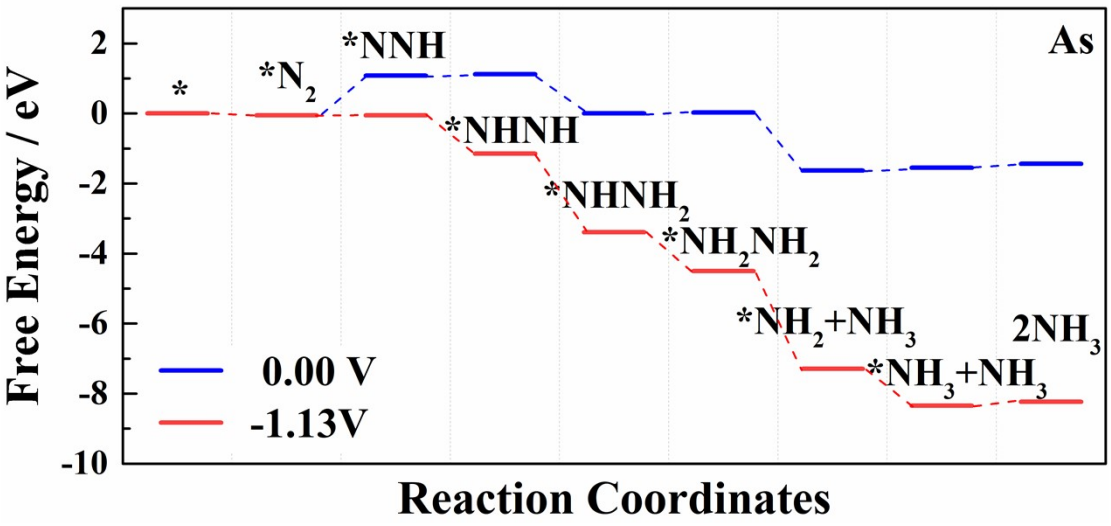


Figure S11. Free energy evolution process for As@GNR system.

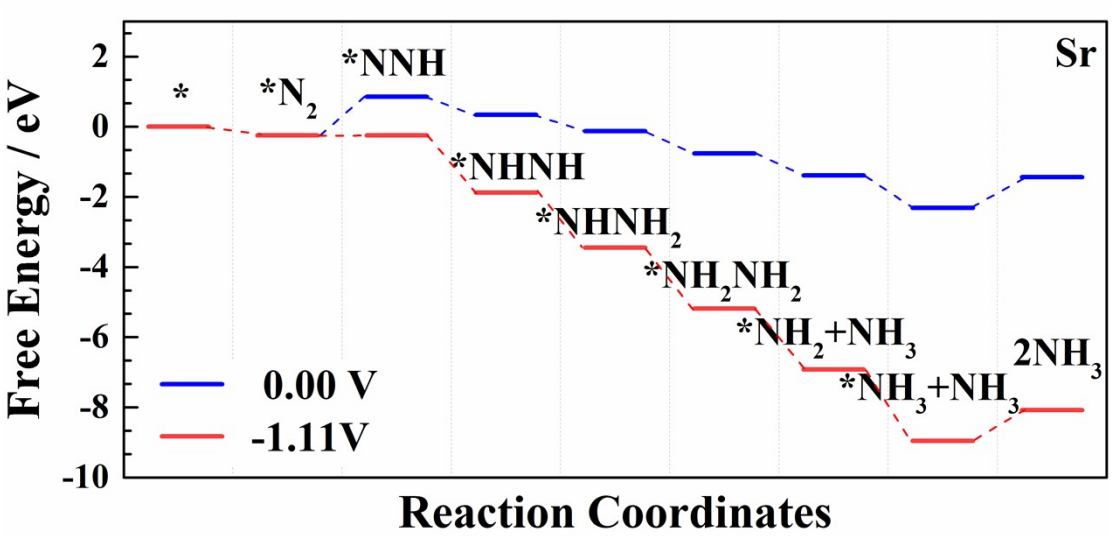


Figure S12. Free energy evolution process for Sr@GNR system.

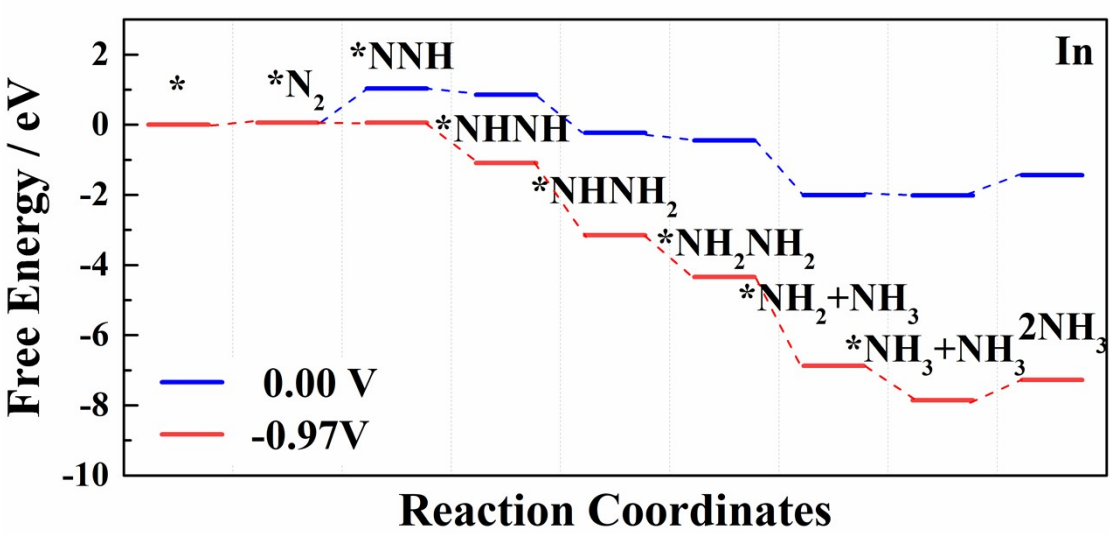


Figure S13. Free energy evolution process for In@GNR system.

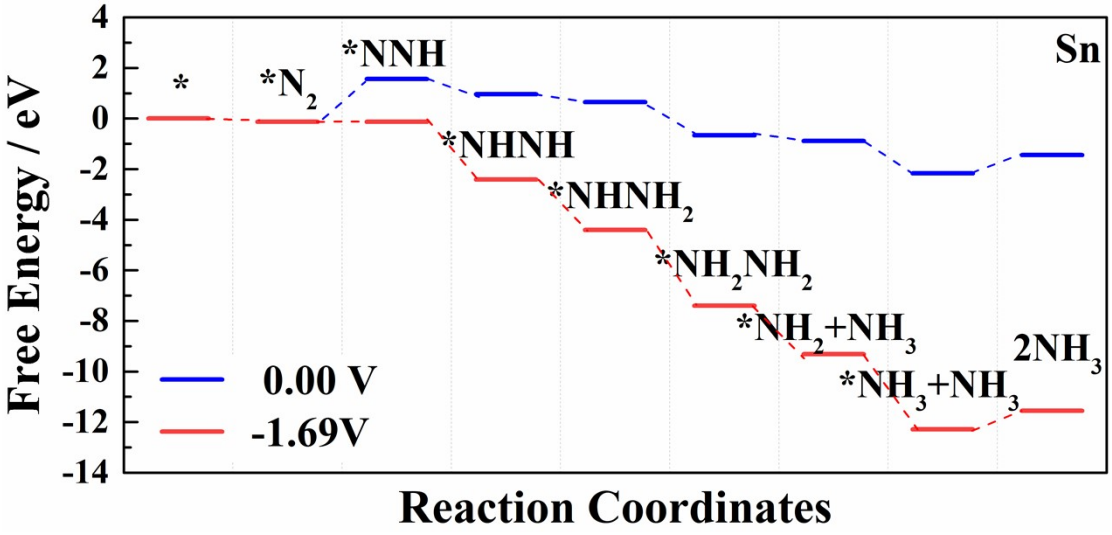


Figure S14. Free energy evolution process for Sn@GNR system.

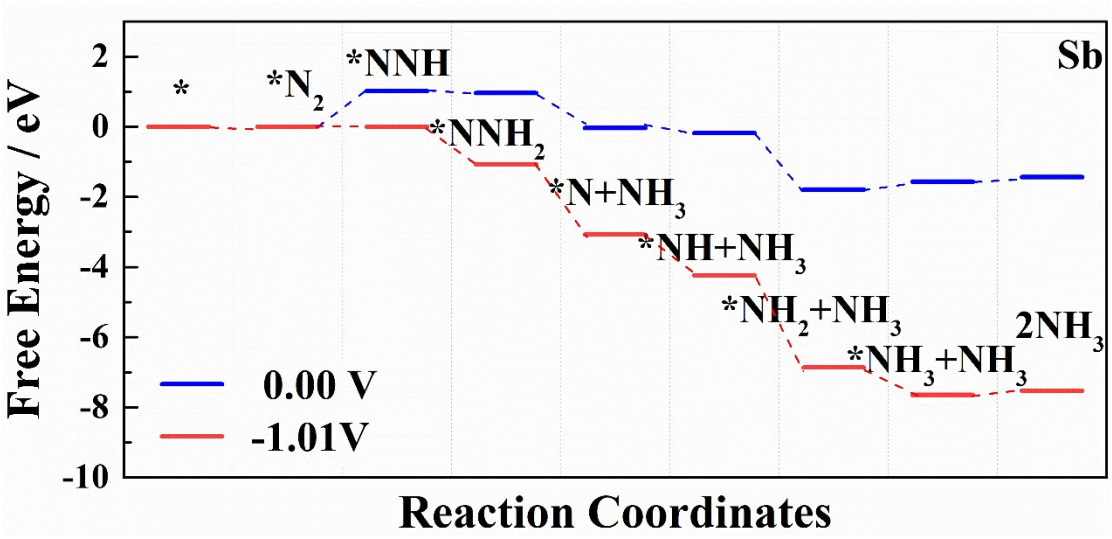


Figure S15. Free energy evolution process for Sb@GNR system.

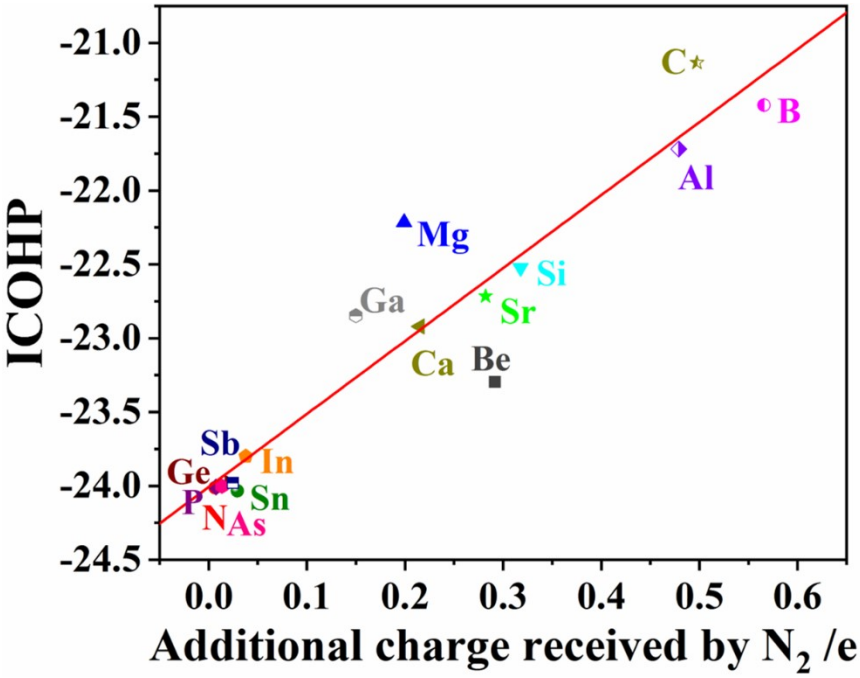


Figure S16. Linear relationship between the amount of charges received by the N_2 and ICOHP of N-N bond after N_2 absorbed on the SAC substrate.

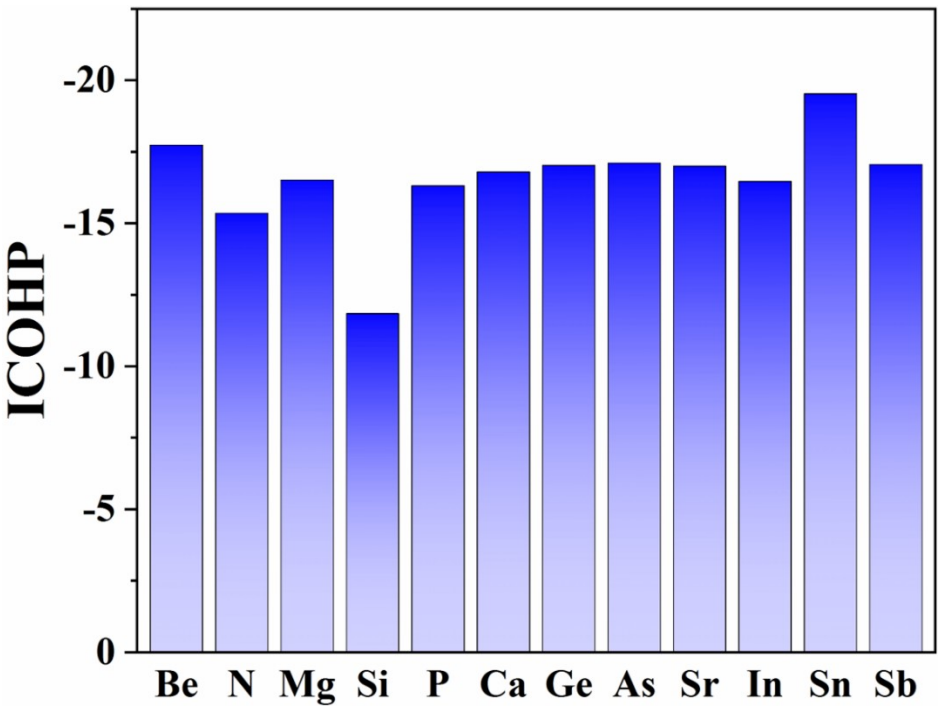


Figure S17. Integrated crystal orbital Hamilton population (ICOHP) of nitrogen-nitrogen bond for SAC-GNR*NNH structure.

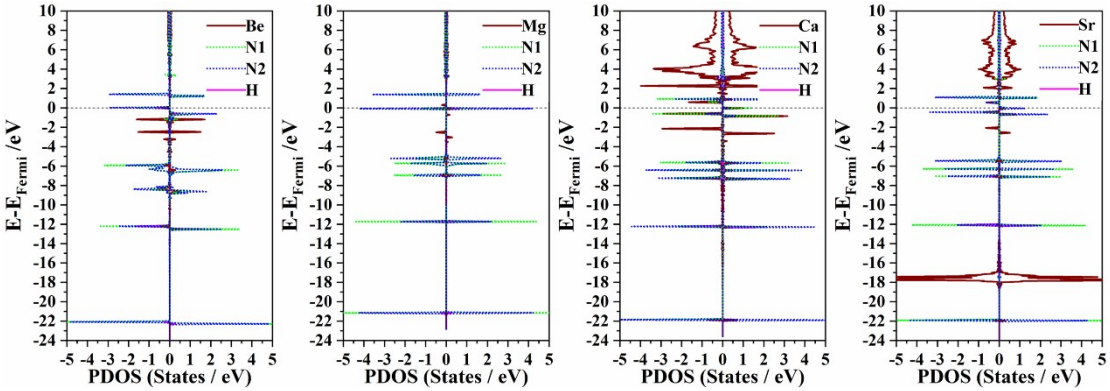


Figure S18. Partial density of states (PDOS) for NNH*Be@GNR, NNH*Mg@GNR, NNH*Ca@GNR and NNH*Sr@GNR structures.

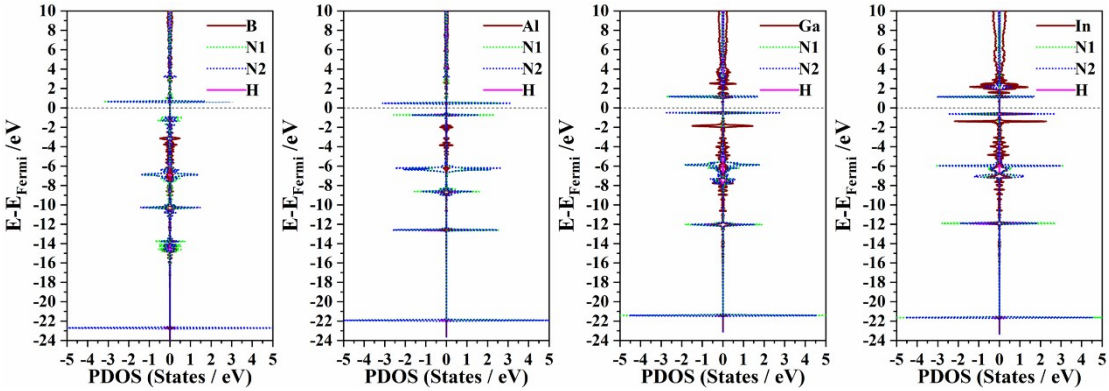


Figure S19. Partial density of states (PDOS) for NNH*B@GNR, NNH*Al@GNR, NNH*Ga@GNR and NNH*In@GNR structures.

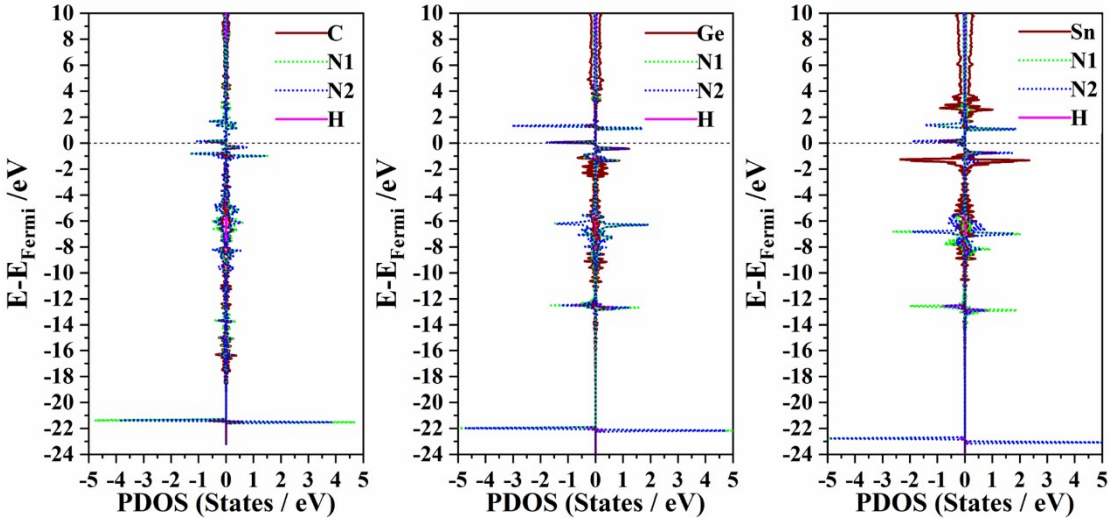


Figure S20. Partial density of states (PDOS) for NNH*C@GNR, NNH*Ge@GNR and NNH*Sn@GNR structures.

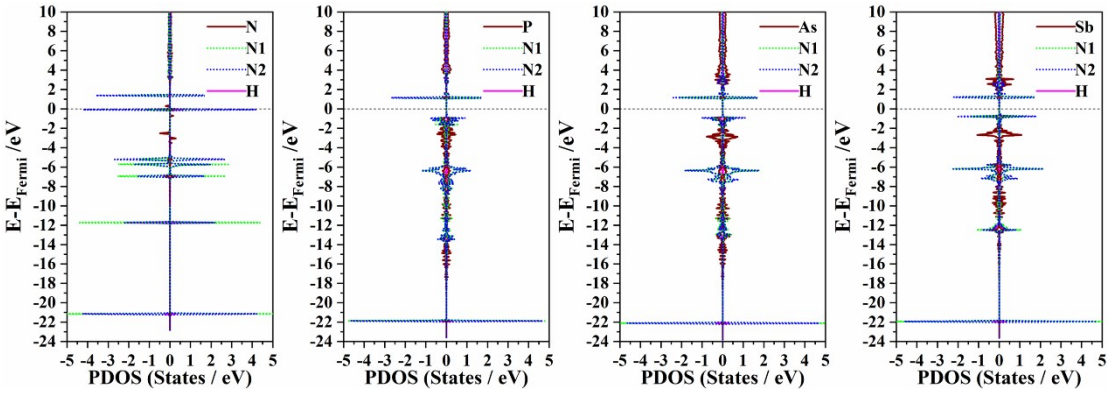


Figure S21. Partial density of states (PDOS) for NNH*N@GNR, NNH*P@GNR, NNH*As@GNR and NNH*Sb@GNR structures.

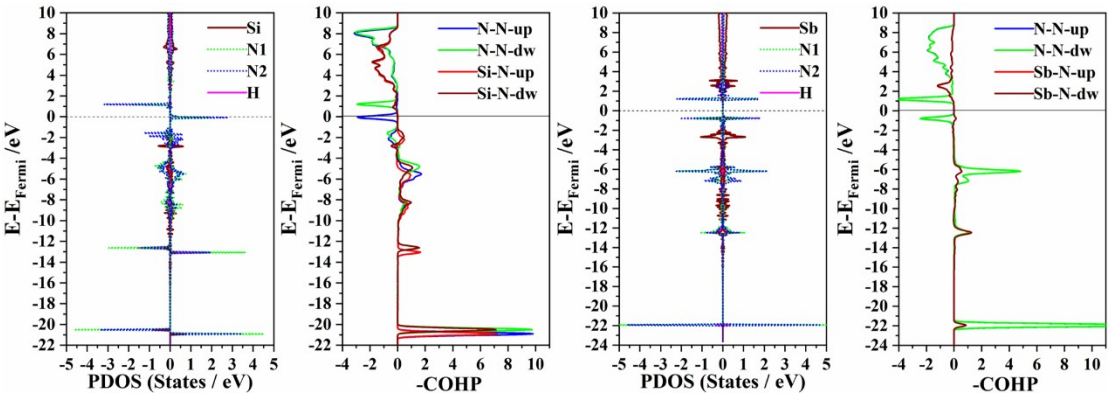


Figure S22. Partial density of states (PDOS) and Crystal occupation Hamilton population (COHP) for NNH*Si@GNR and NNH*Sb@GNR structures.

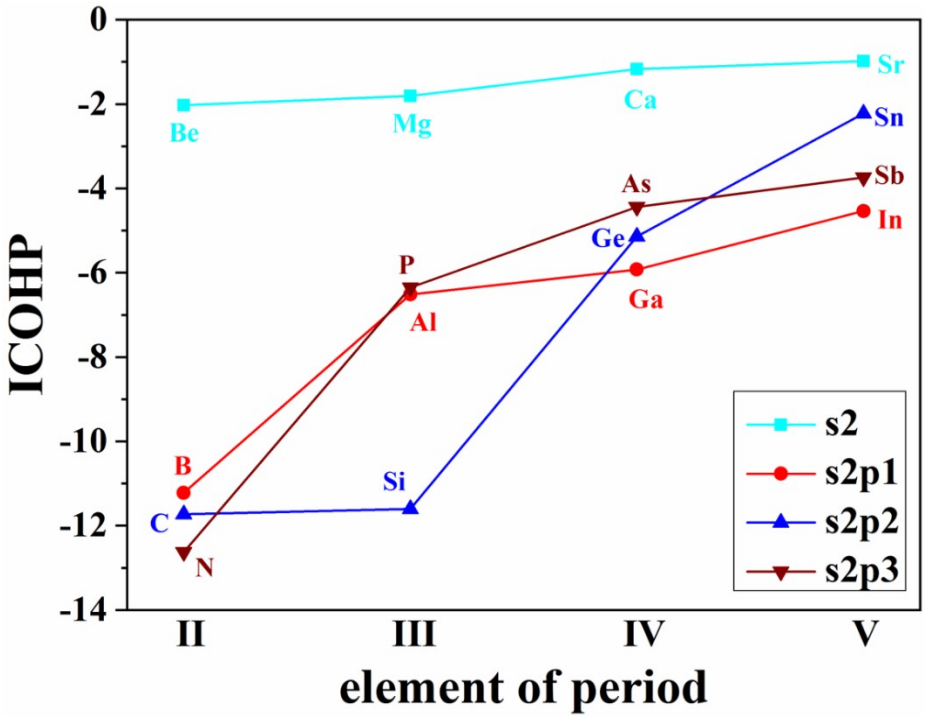


Figure S23. Integrated crystal orbital Hamilton population (ICOHP) of all SAC@GNR systems

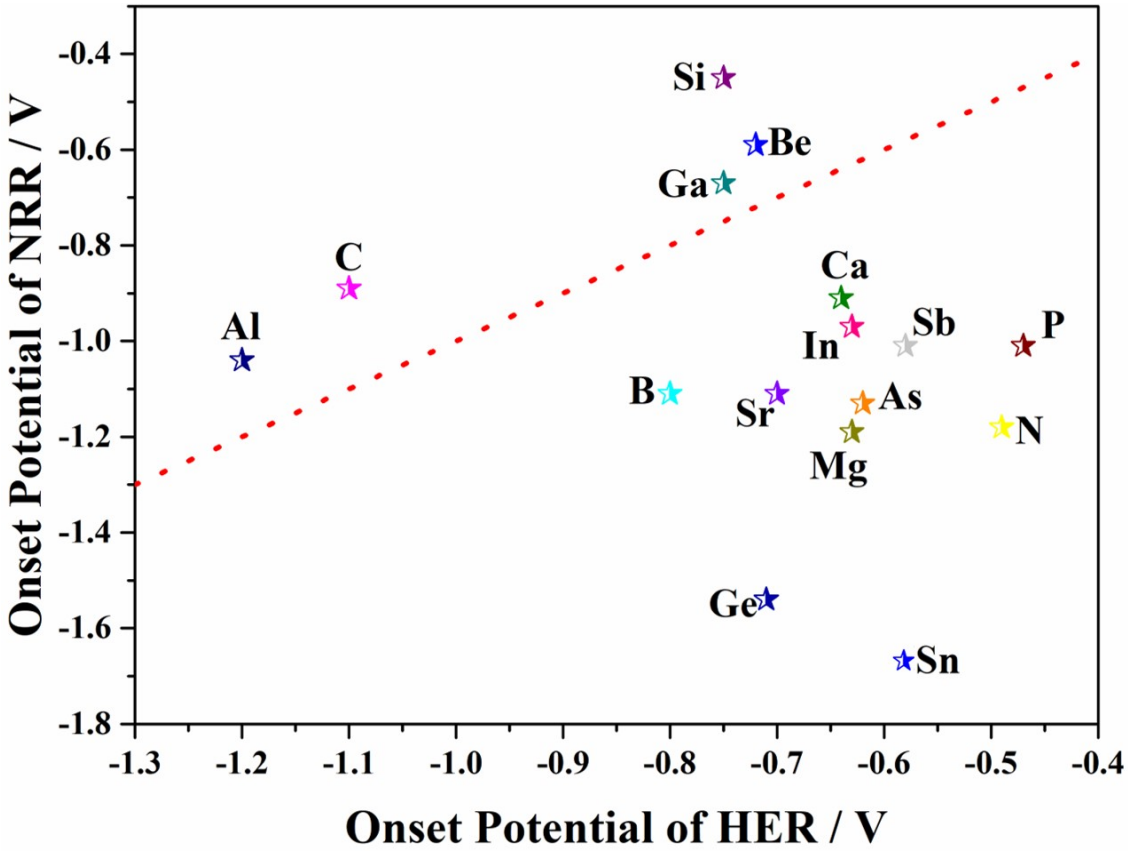


Figure S24. The comparison of the electrochemical performance for NRR and HER process. The dashed line represents HER and NRR share equal onset potentials while for elements below this line, the HER performance prevails NRR.