Supporting Information

Strain Engineering: an efficient strategy to enhance the catalytic activity of SACs on waved graphene for e-NRR

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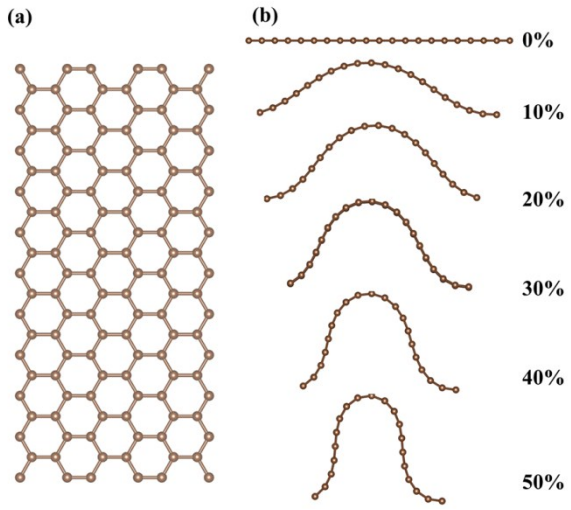

Figure S1.Top view of flat graphene (a) and side views (b) of waved-graphene with different curvatures.

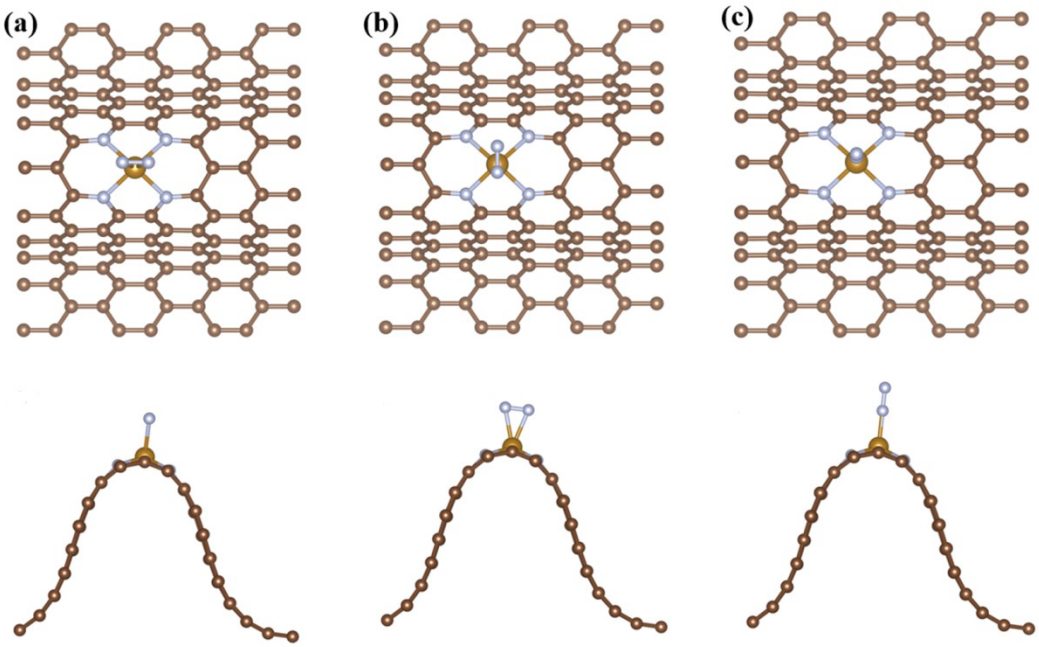

Figure S2. There are three stable adsorption configurations, which are named as a-adsorption (side-on) (a), b-adsorption (side-on) (b) and c–adsorption (end-on) (c).

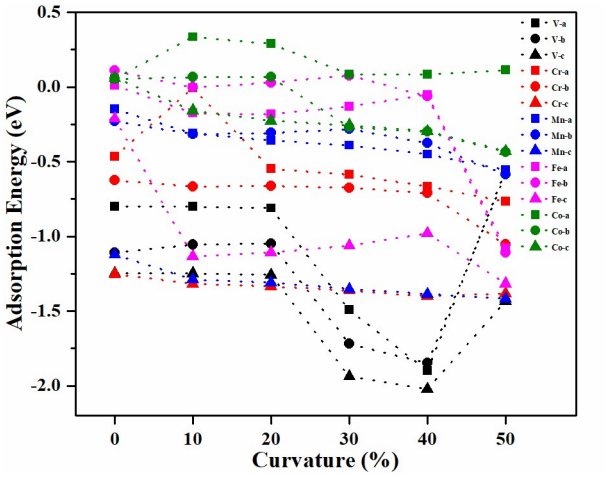

Figure S3. The adsorption energies of different adsorption configurations of SACs-wG.

Table S1. Adsorption energy and adsorption length of N_2 adsorbed SAC-Cu-wG and SAC-Pt-wG.

Curvature (%)	Adsorption energy (meV)		Adsorption length (Å)	
	SAC-Cu-wG	**SAC-Pt-wG**	**SAC-Cu-wG**	**SAC-Pt-wG**
0	**-80**	**-89**	**3.07**	**3.69**
10	**-63**	**-59**	**3.35**	**3.48**
20	**-60**	**-60**	**3.04**	**3.71**
30	**-63**	**-66**	**3.23**	**3.76**
40	**-52**	**-55**	**3.14**	**3.44**
50	**-54**	**-60**	**3.09**	**3.38**

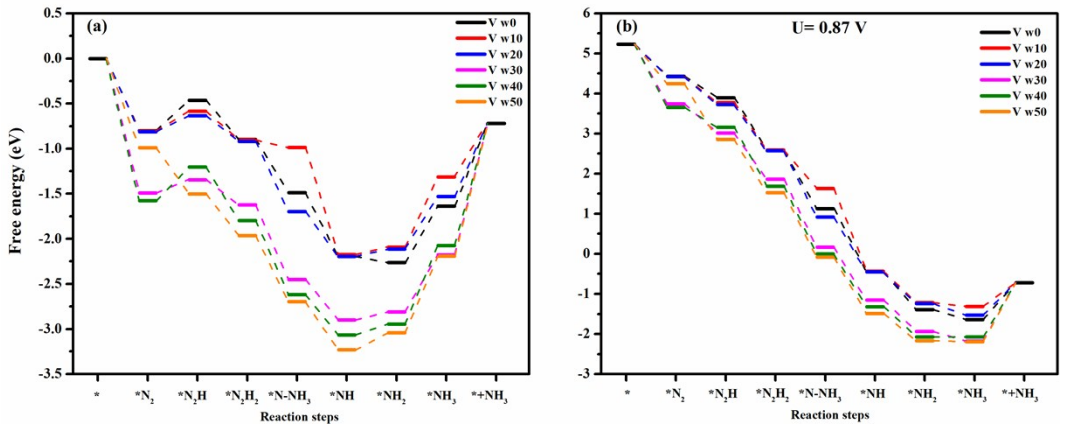

Figure S4. Free energy diagrams for the e-NRR progresses on SAC-V-wG at U= 0 and U= 0.87 V

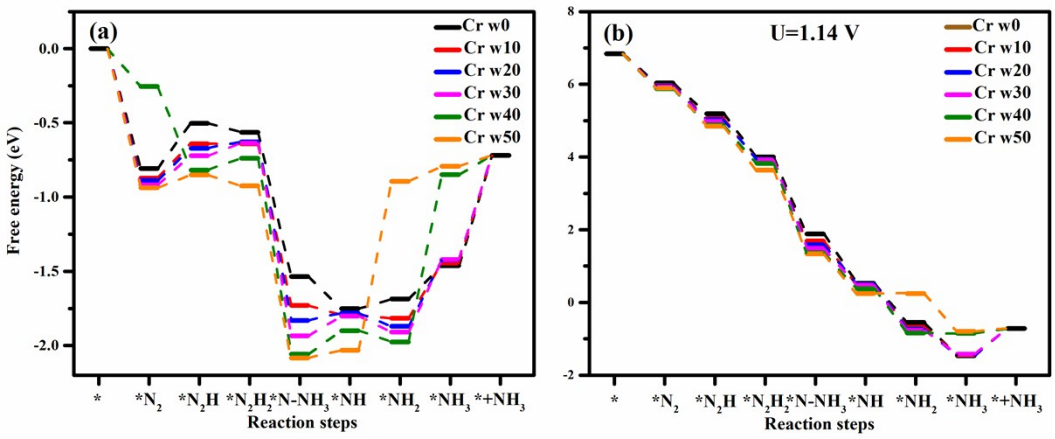

Figure S5. Free energy diagrams for the e-NRR progresses on SAC-Cr-wG at U= 0 and U= 1.14V

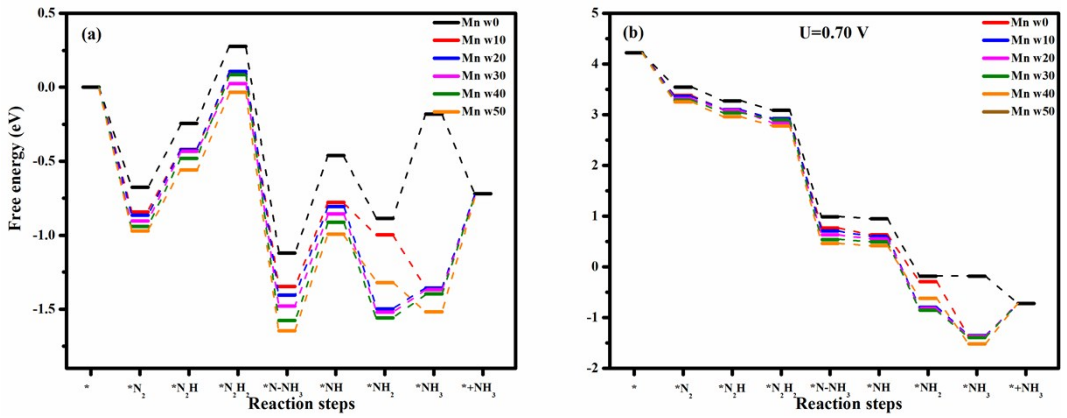

Figure S6. Free energy diagrams for the e-NRR progresses on SAC-Mn-wG at U= 0 and U= 0.70 V

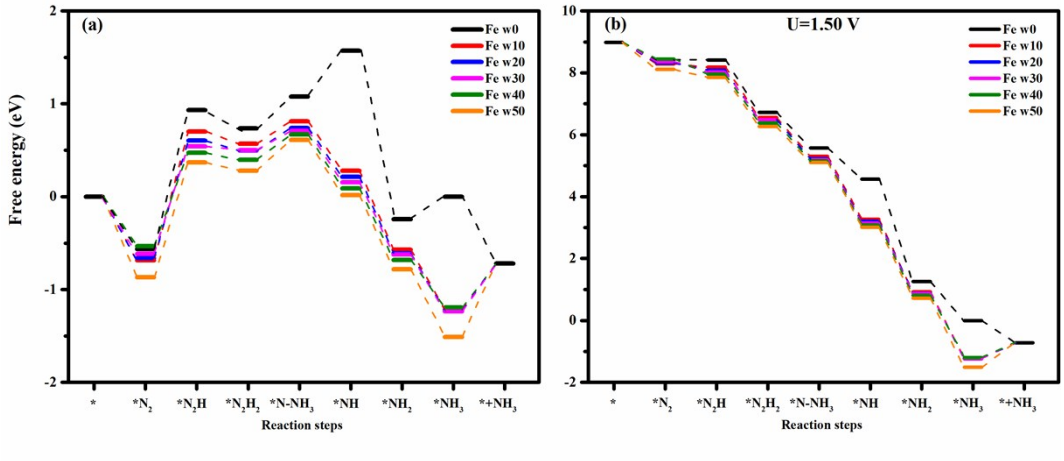

Figure S7. Free energy diagrams for the e-NRR progresses on SAC-Fe-wG at U= 0 and U= 1.50 V

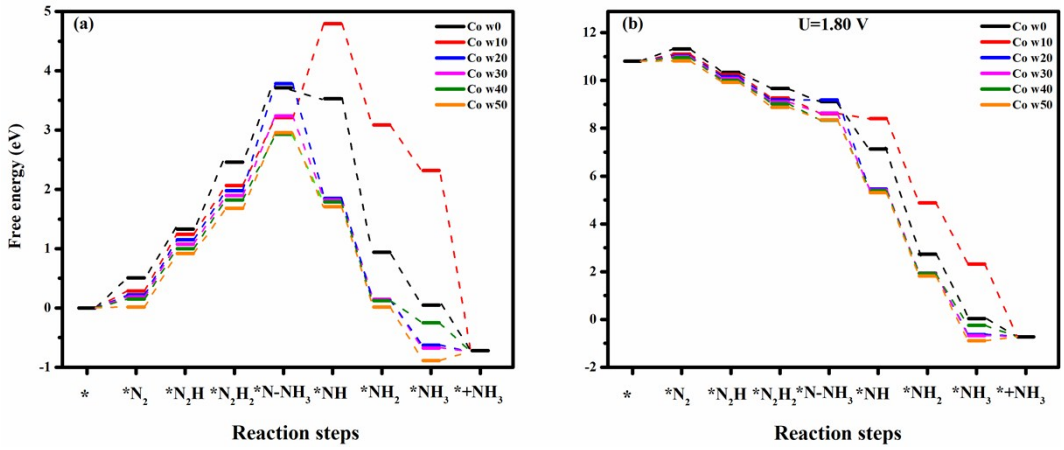

Figure S8. Free energy diagrams for the e-NRR progresses on SAC-Co-wG at U= 0 and U= 1.80 V

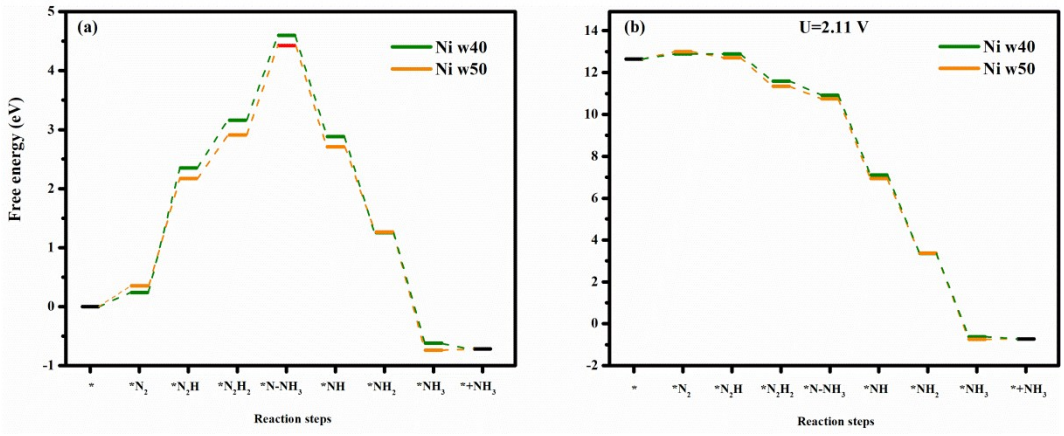

Figure S9. Free energy diagrams for the e-NRR progresses on SAC-Ni-wG at U= 0 and U= 2.11 V

Table S2. ΔG_{RDS} (eV) of SACs-wG

Curvature (%)	SAC-V-wG	SAC-Cr-wG	SAC-Mn-wG	SAC-Fe-wG	SAC-Co-wG	SAC-Ni-wG
0	0.63	0.30	0.70	1.50	1.03	
10	0.78	0.37	0.57	1.39	1.58	
20	0.58	0.45	0.60	1.26	1.80	
30	0.63	0.49	0.62	1.16	1.34	
40	0.87	0.91	0.66	1.01	1.11	2.11
50	0.85	1.14	0.66	1.24	1.28	1.82

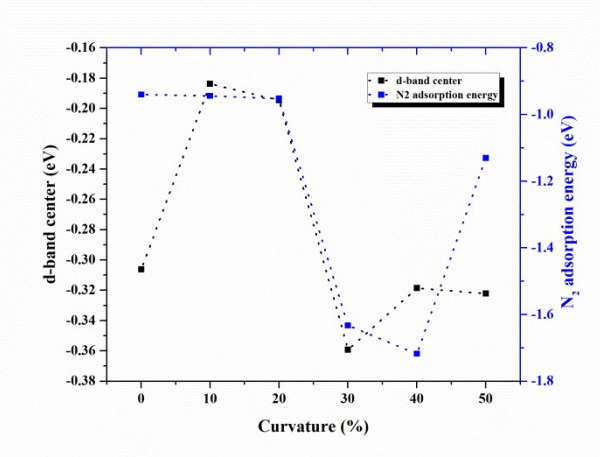

Fig S10. The d-band centers and N2 adsorption energies of SAC-V-wG at different curvatures

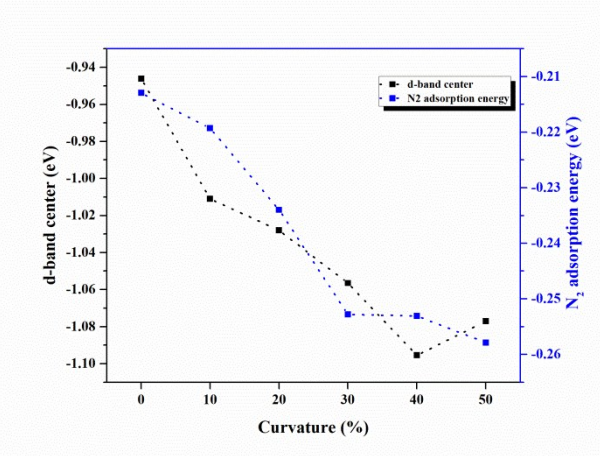

Fig S11. The d-band centers and N2 adsorption energies of SAC-Cr-wG at different curvatures

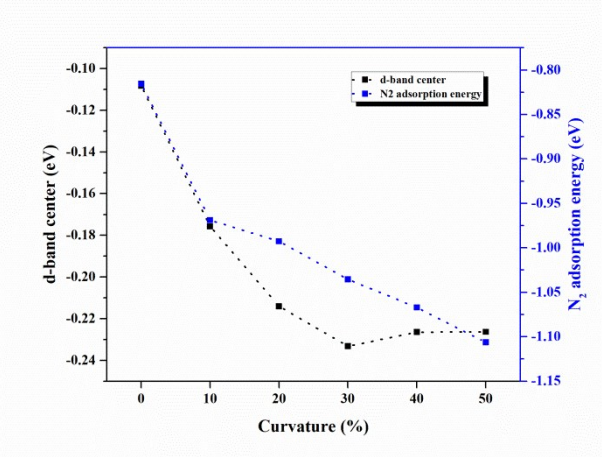

Fig S12. The d-band centers and N2 adsorption energies of SAC-Mn-wG at different curvatures