Supplementary Information (SI) for RSC Advances.
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Theoretical study of a CuCo dual-atom catalyst for nitrogen fixation

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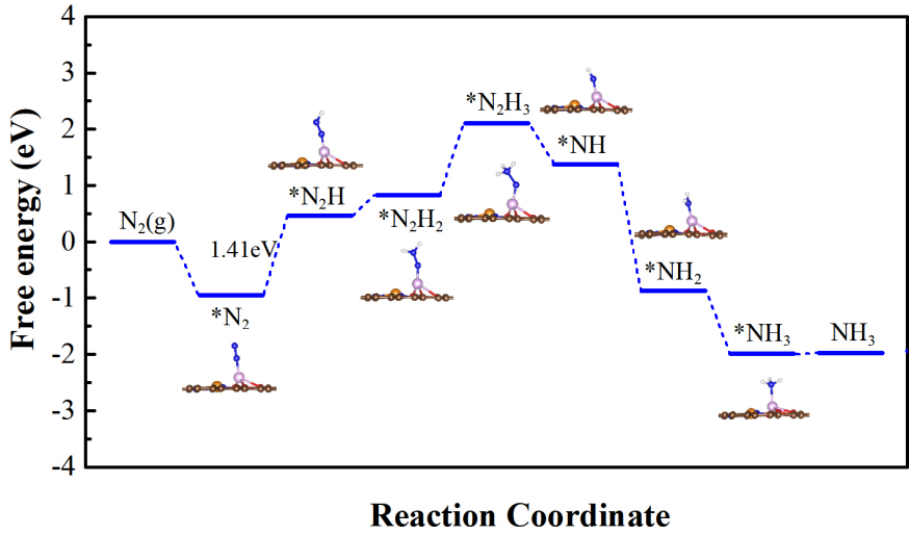

Fig. S1. Free energy diagram along the reaction path of NRR proceeded on N-CuCo-O starting with N_2 adsorbed on Co site.

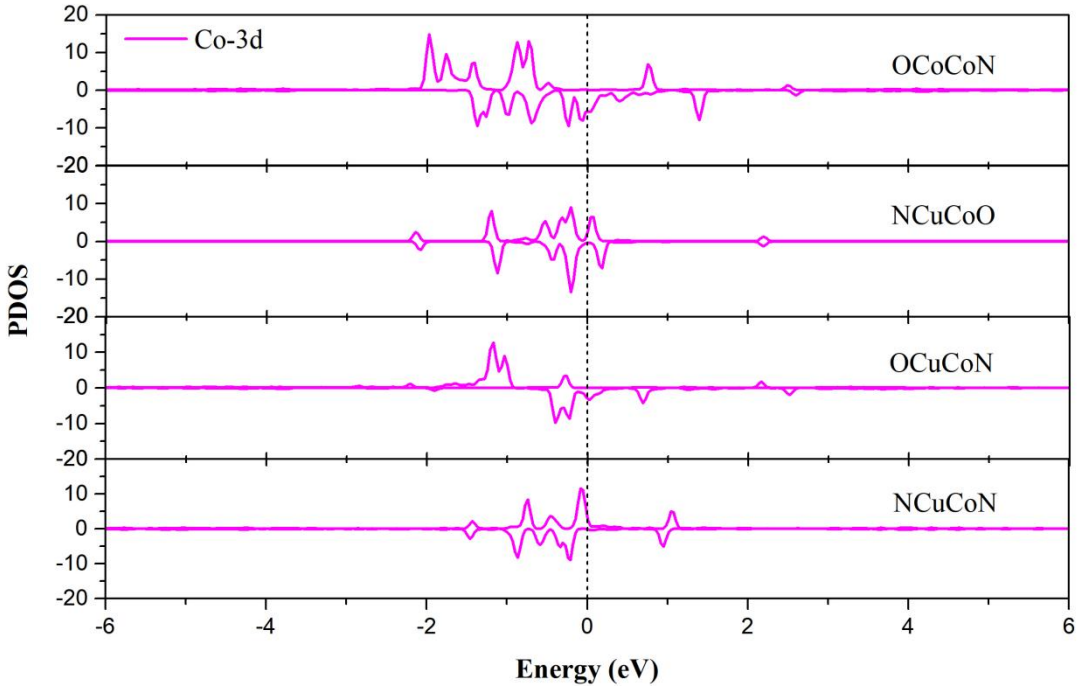

Fig. S2. The projected density of states of Co-3d in different configurations.

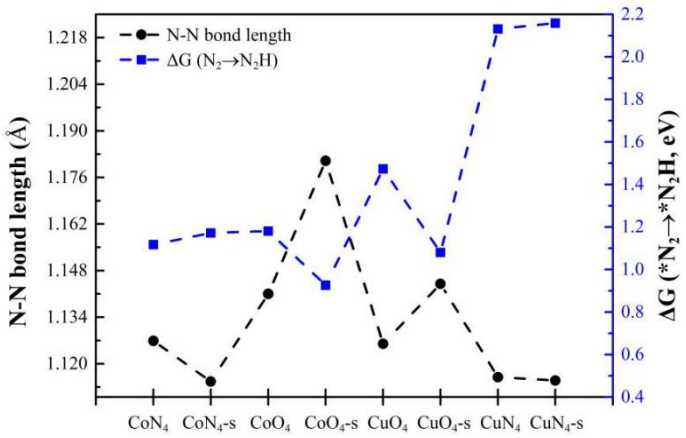

Fig. S3. The relationship between N-N bond length of adsorbed $*N_2$ and Gibbs free energy change ΔG from $*N_2$ to $*N_2H$ on different SACs.

Table SI. calculated energy(E), zero point energy(ZPE) and contribution from entropy(TS) of O-CuCo-N DAC.

O-CuCo-N (side-on)	E	ZPE	TS
$*N_2$	-639.300	0.204	0.106
*NNH-Cu	-642.549	0.530	0.084
*NNH-Co	-642.289	0.530	0.084
*NHNH	-646.228	0.835	0.11
$*NNH_2$	-645.308	0.826	0.123
$*NH_2NH$	-649.771	1.149	0.160
$*NH_2NH_2$	-654.360	1.319	0.179
$*NH_2NH_3$	-659.042	1.700	0.228
$*NH_3$	-642.495	1.04	0.10
$*NH_3NH_3$	-662.789	2.074	0.198
O-CuCo-N (end-on)	E	ZPE	TS
*Co-N_2	-639.306	0.196	0.160
$*N_2H$	-642.318	0.506	0.120
$*N_2H_2$	-646.008	0.820	0.139
$*N_2H_3$	-648.798	1.159	0.154
*NH	-634.440	0.341	0.089
$*NH_2$	-639.233	0.713	0.076

*NH_3	-642.492	1.018	0.127

Table SII calculated energy(E), zero point energy(ZPE) and contribution from entropy(TS) of O-CoCo-O DAC.

O-CoCo-O (side-on)	Energy	ZPE	TS
*N_2	-631.469	0.203	0.106
*N_2H	-634.771	0.513	0.098
*NHNH	-638.346	0.889	0.346
*NH_2N	-637.697	0.829	0.121
*NH_2NH	-641.992	1.134	0.167
*NH_2NH_2	-646.944	1.309	0.261
*NH_3NH	-646.468	1.280	0.216
*NH_3NH_2	-651.269	1.683	0.229
*NH_3NH_3	-654.432	2.032	0.323