Supporting Information for

Cu@g-C_3N_4: An Efficient Single Atom Electrocatalyst for NO Electrochemical Reduction with Suppressed Hydrogen Evolution

Qian Wu, Wei Wei,* Xingshuai Lv, Yuanyuan Wang, Baibiao Huang, Ying Dai*

School of Physics, State Key Laboratory of Crystal Materials, Shandong University, Jinan 250100, China

*Email: weiw@sdu.edu.cn (W. Wei); daiy60@sina.com (Y. Dai)

Table S1 Charge transfer of TM atoms after adsorption on g-C_3N_4 by bader charge analysis.

	V	Cr	Mn	Fe	Co	Ni	Cu	Mo
ΔQ (eV)	1.288	1.257	1.311	0.979	0.770	0.745	0.753	1.114

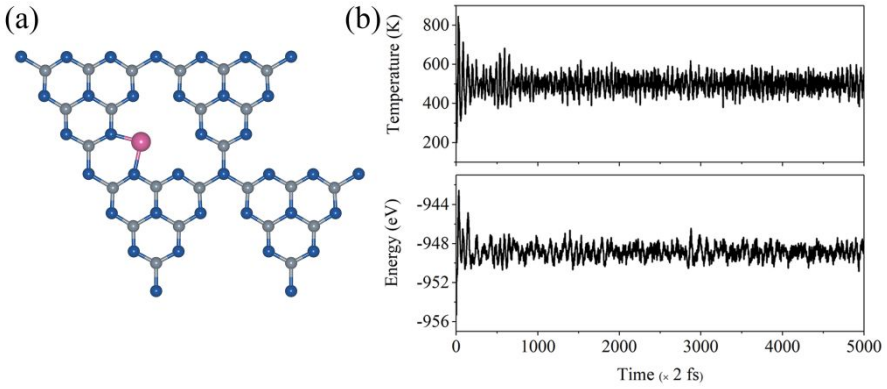

Fig. S1 (a) Optimized structure of Cu@g-C_3N_4. (b) Variation of temperature and total energy for Cu@g-C_3N_4 during AIMD simulation. The simulation was running under 500 K for 10 ps with a time step of 2 fs. Gray, blue and pink balls represent C, N, and Cu atoms, respectively.

Table S2 Calculated reaction energy, zero-point energy, entropy and Gibbs free energy of different

species adsorbed Cu@g-C_3N_4. The unit is eV.

	E	*ZPE*	*TS*	*G*
*HNO + Cu@ g-C_3N_4	-495.025	0.651	0.022	-494.396
*NOH+ Cu@ g-C_3N_4	-493.919	0.666	0.022	-493.275
*HNOH+ Cu@ g-C_3N_4	-498.570	0.957	0.095	-497.708
$^*H_2NO$+ Cu@ g-C_3N_4	-498.833	1.004	0.026	-497.855
*N+ Cu@ g-C_3N_4	-482.590	0.176	0.007	-482.421
$^*H_2NOH$+ Cu@ g-C_3N_4	-503.525	1.355	0.027	-502.197
*NH+ Cu@ g-C_3N_4	-487.869	0.424	0.036	-487.481
$^*NH_2$+ Cu@ g-C_3N_4	-493.548	0.753	0.058	-492.853
$^*NH_3$+ Cu@ g-C3N4	-498.325	1.131	0.052	-497.246
NH_3 (g) + Cu@ g-C_3N_4	-496.760	1.074	0.158	-495.844

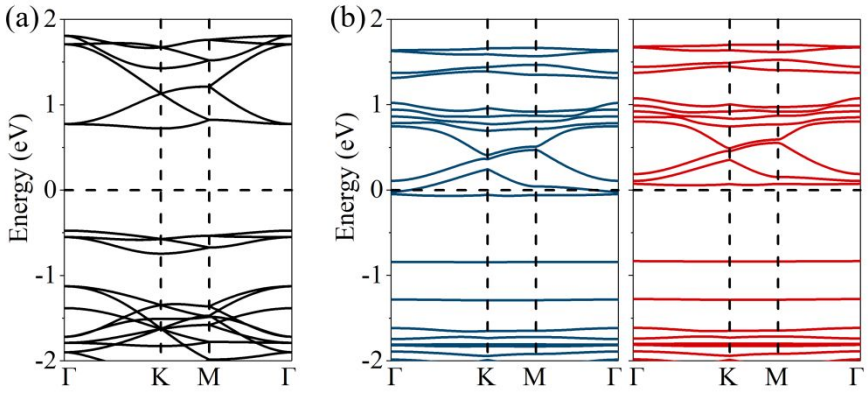

Fig. S2 Band structures of (a) initial g-C_3N_4 and (b) Cu@g-C_3N_4. Blue and red lines indicate majority and minority spin band structures. The Fermi level is set to zero.

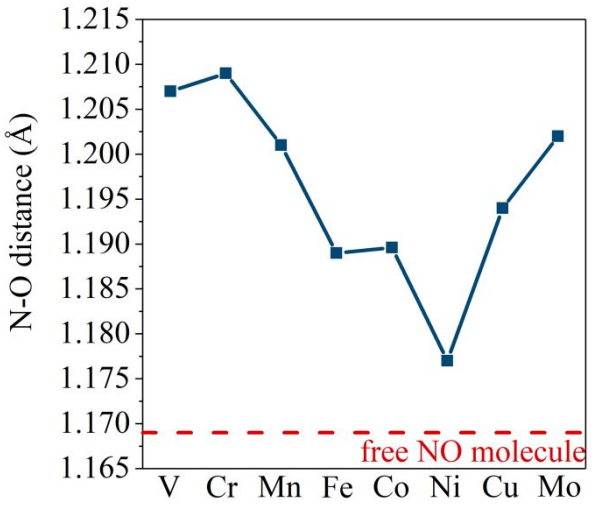

Fig. S3 N–O bond length of adsorbed NO molecule on different TM atoms decorated g-C_3N_4. The red dash line indicates the initial N–O bond length of free NO molecule.

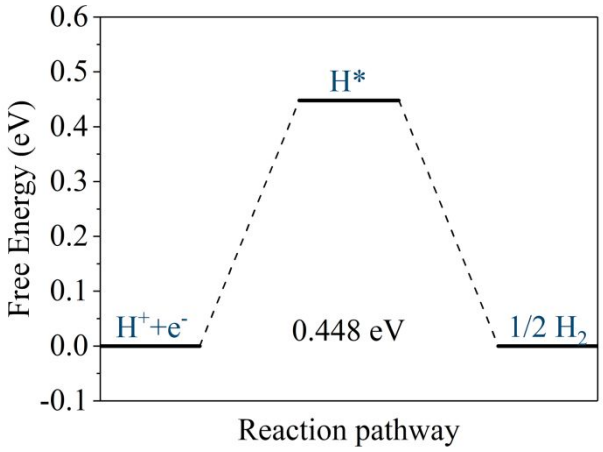

Fig. S4 Gibbs free energy diagram of Cu@g-C_3N_4 for HER.