Supplementary Materials

Design of Fe_2Mo@γ-GDY triatomic catalyst for electrocatalytic urea synthesis of N_2 and CO: a theoretical study

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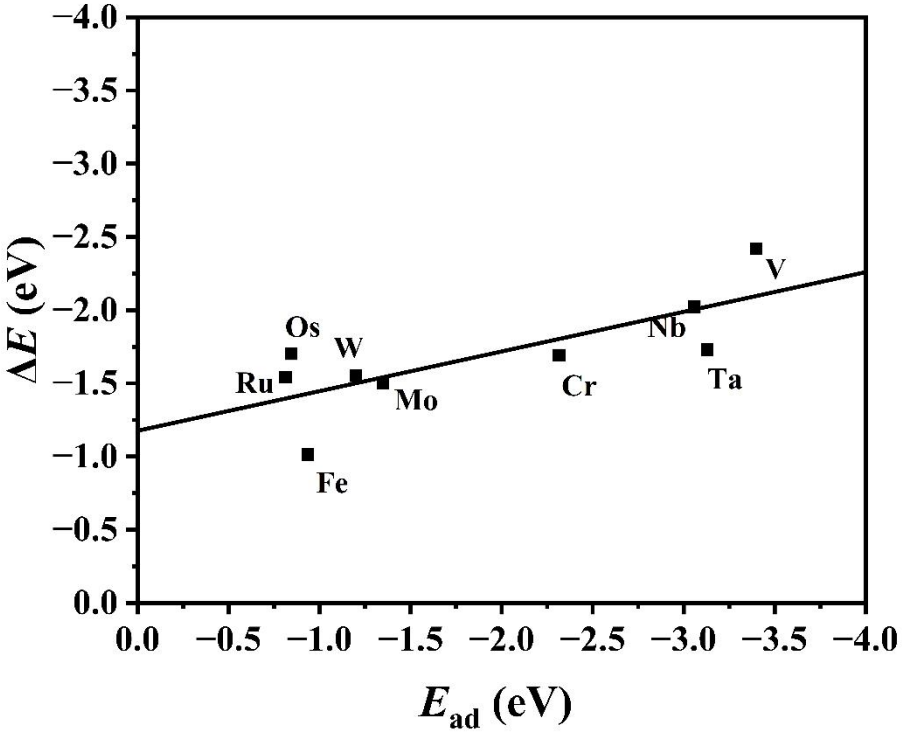
Formula:

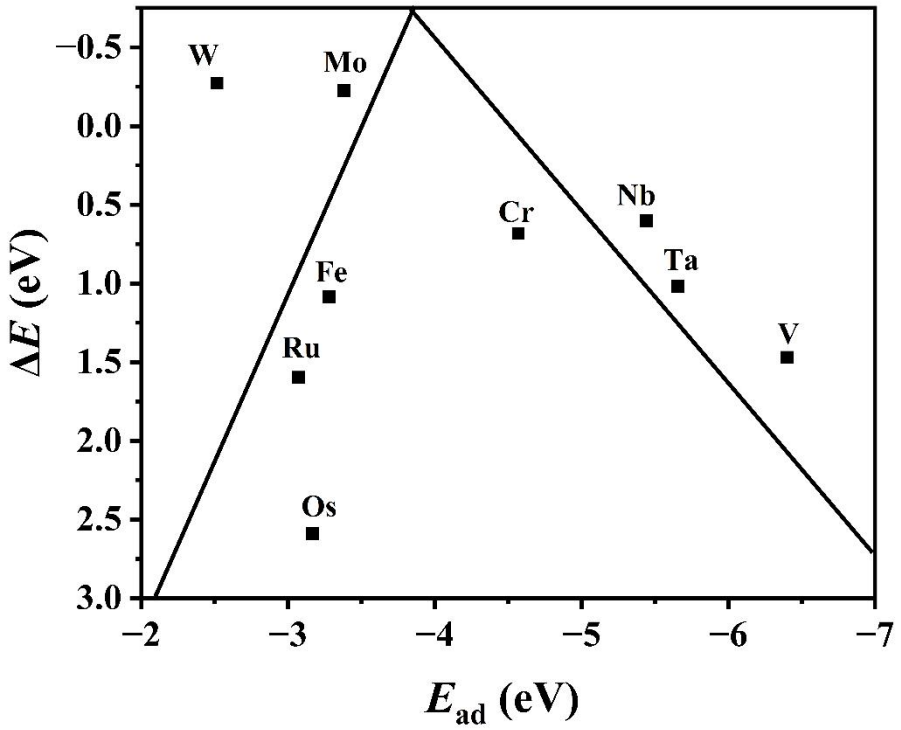
To evaluate the stability of the system, the formation energy is evaluated by:

$$E_{form} = E_{total} - E_{GDY} - 2E_{Fe} - E_{Mo}$$

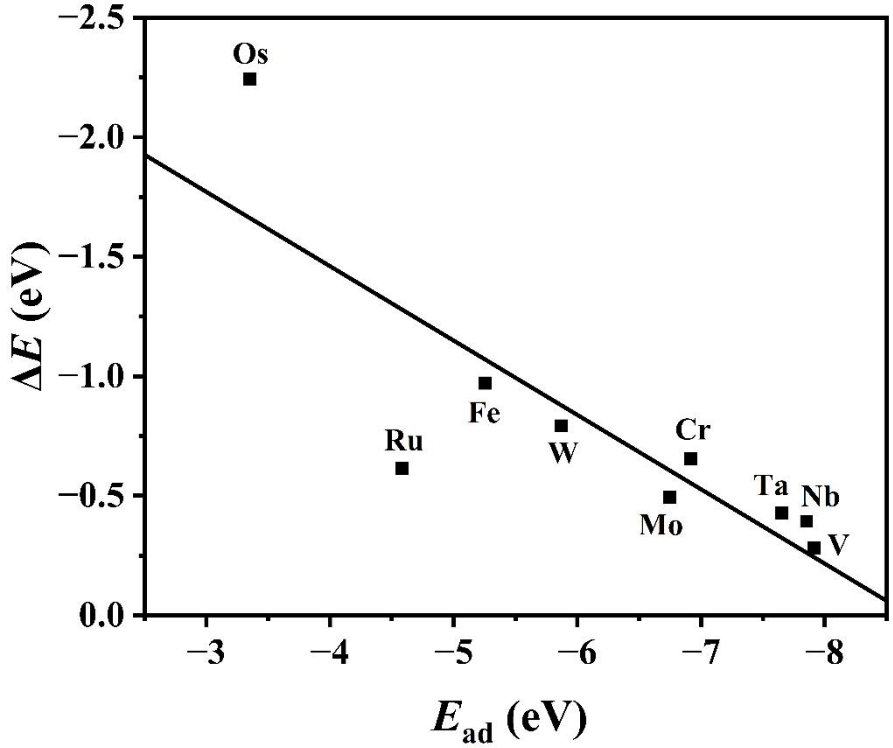
where E_{total}, E_{GDY}, E_{Fe}, and E_{Mo} represent the energy of entire structure, the energy of GDY, the energy of a single Fe atom, the energy of a single Mo atom, respectively.



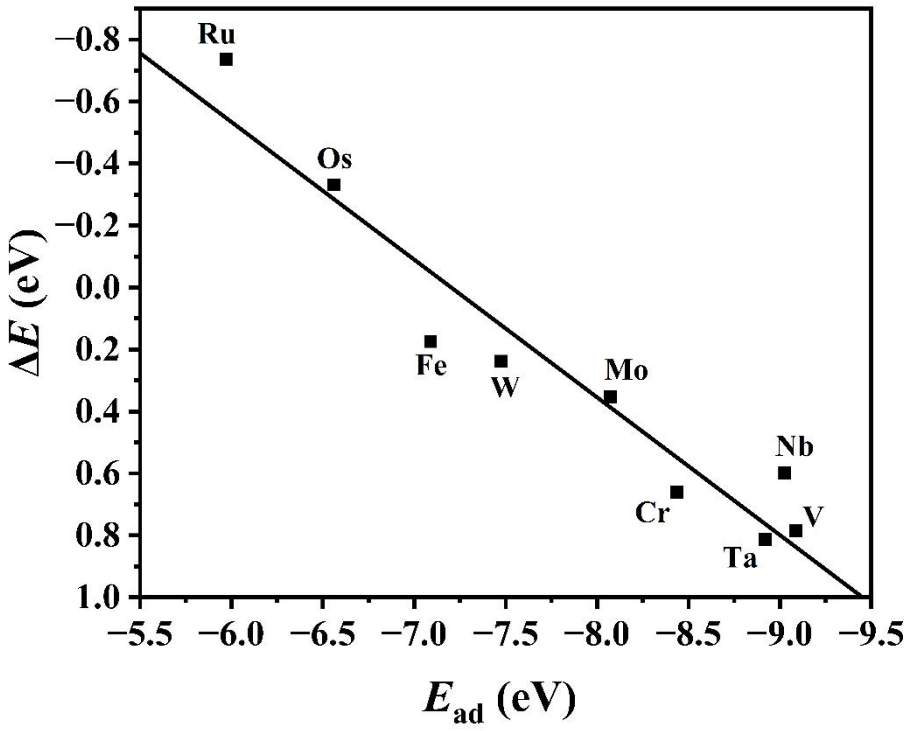
Supplementary Figure 1. E_{ad}-ΔE curve of *N_2-*N_2+*CO step.



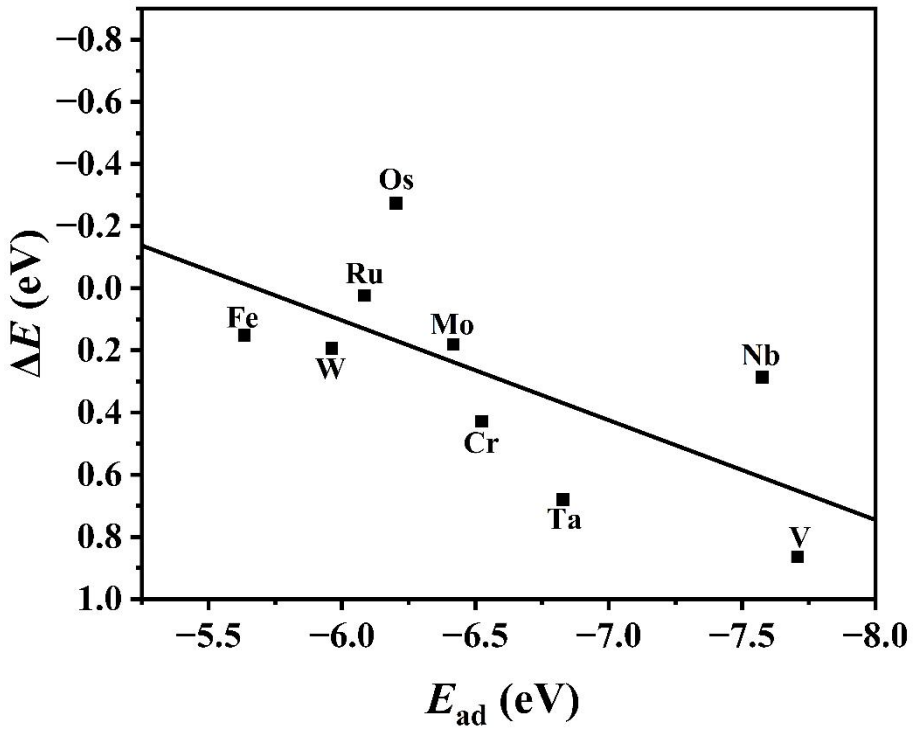
Supplementary Figure 2. E_{ad}-ΔE curve of *N_2+*CO-*NCON step.



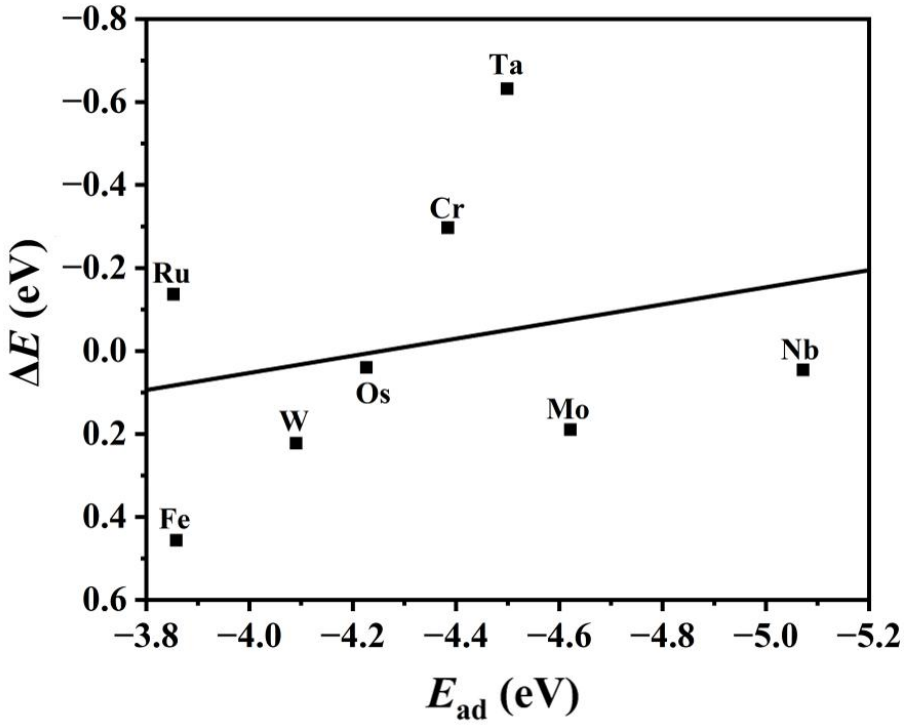
Supplementary Figure 3. E_{ad}-ΔE curve of *NCON-*NCONH step.



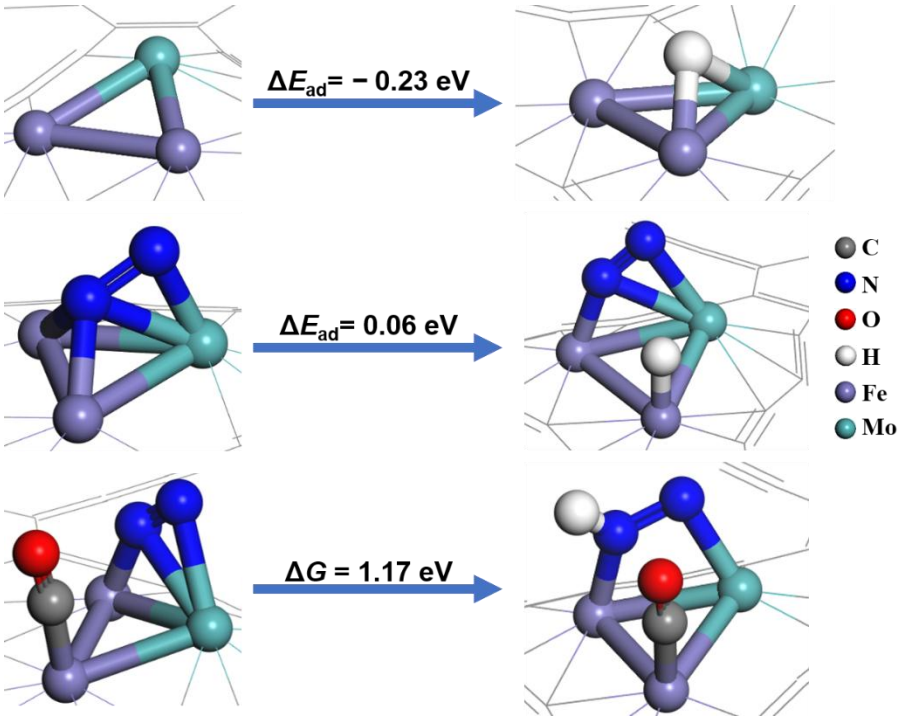
Supplementary Figure 4. E_{ad}-ΔE curve of *NCONH-*$NCONH_2$ step.



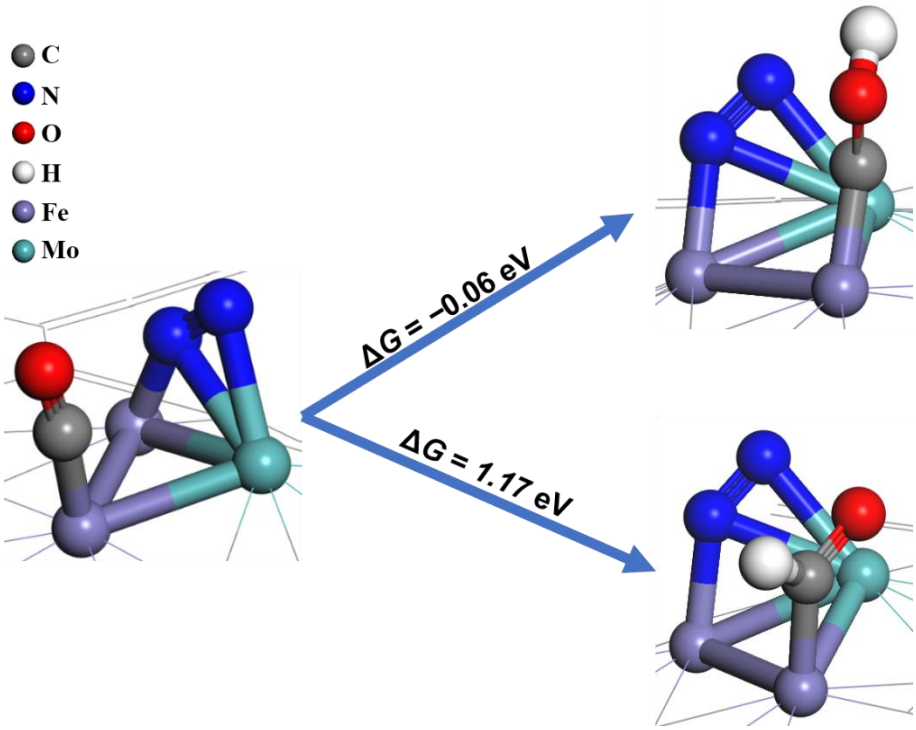
Supplementary Figure 5. E_{ad}-ΔE curve of *$NCONH_2$-*$HNCONH_2$ step.



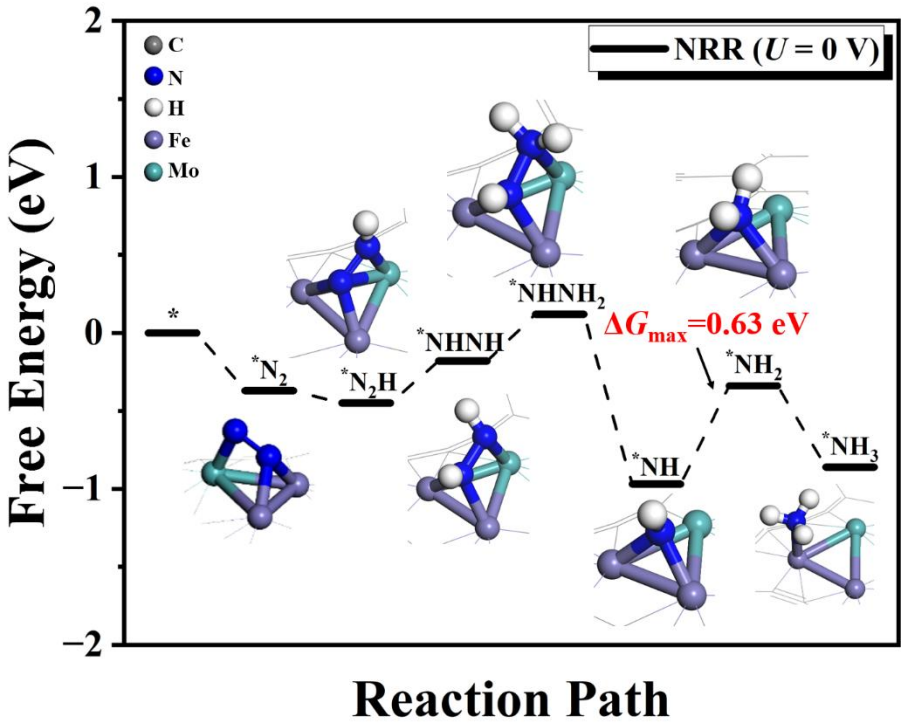
Supplementary Figure 6. E_{ad}-ΔE curve of *$HNCONH_2$-*H_2NCONH_2 step.



Supplementary Figure 7. Structure of HER.



Supplementary Figure 8. Structure of CORR.



Supplementary Figure 9. Evolution of free energy of NRR.

Supplementary Table 1. Hirshfeld charge of structures

Structure	Hirshfeld charge on N1	Hirshfeld charge on N2
Fe_3@γ-GDY-*NCON	−0.18	−0.20
Fe_2Mo@γ-GDY-*NCON	−0.22	−0.25
$FeMo_2$@γ-GDY-*NCON	−0.24	−0.24
Mo_3@γ-GDY-*NCON	−0.24	−0.26