

Supporting Information

Theoretical exploration of the nitrogen fixation mechanism of two-dimensional dual-metal FeTM@GY (TM=Fe, Mo, Co, and V) electrocatalysts

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Table S1 Binding energy (E_b) of FeTM@GY (TM = Fe, Mo, Co, and V), bond lengths of Fe and TM atoms $d_{\text{Fe-TM}}$, average values of bond lengths of Fe and TM atoms to C atoms $\bar{d}_{\text{Fe-C}}$ and $\bar{d}_{\text{TM-C}}$, respectively, and bond lengths between Fe and TM atoms to GY Bader charge transfer Q_{Fe} and Q_{TM} .

	E_b (eV)	$d_{\text{Fe-TM}}$ (Å)	$\bar{d}_{\text{Fe-C}}$ (Å)	$\bar{d}_{\text{TM-C}}$ (Å)	Q_{Fe} (e)	Q_{TM} (e)
FeFe@GY	-2.92	2.20	2.00	1.99	-0.56	-0.58
FeMo@GY	-3.49	2.12	1.98	2.09	-0.40	-0.83
FeCo@GY	-2.66	2.20	2.00	1.96	-0.67	-0.40
FeV@GY	-2.90	2.04	1.97	2.08	-0.31	-1.00

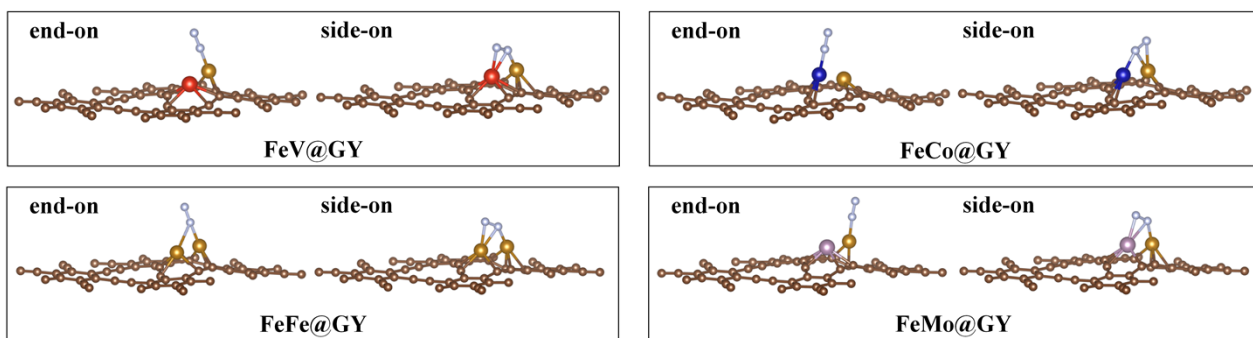


Fig. S1 Optimized structures of N₂ molecules adsorbed on FeTM@GY (TM = Fe, Mo, Co, and V) via end-on and side-on configurations.

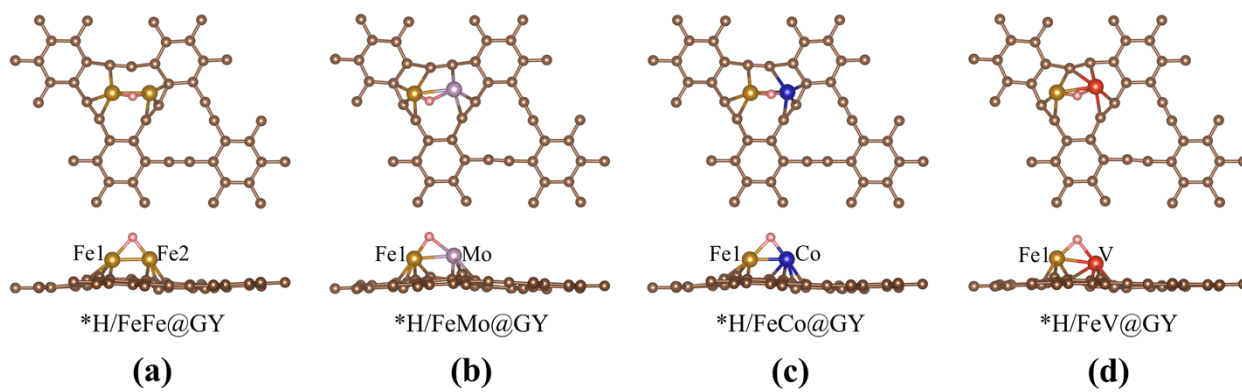


Fig. S2 Optimized structures of H atom adsorption on FeTM@GY: (a) Fe, (b) Mo, (c) Co and (d) V.

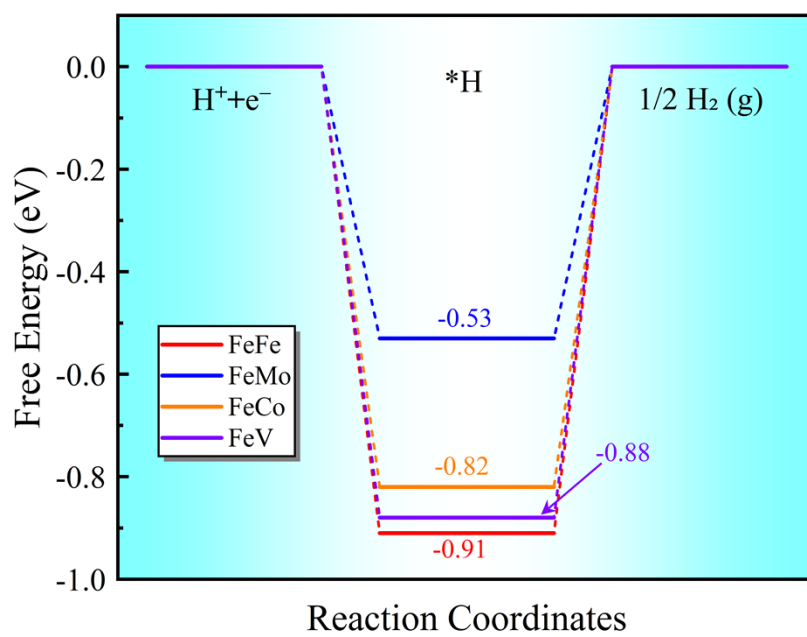


Fig. S3 Gibbs free energy diagram of H^+ on FeTM@GY (TM = Fe, Mo, Co, V) for HER.

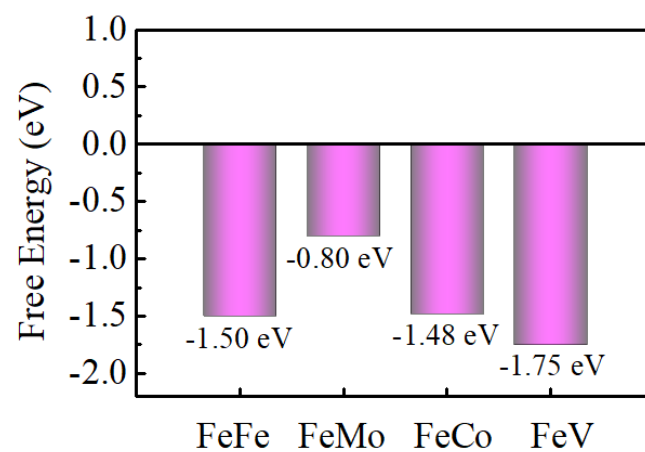


Fig. S4 Free energies of *H [$\Delta G(*H)$] adsorption on FeFe, FeMo, FeCo, and FeV@GY under the corresponding electrode potential of -0.59, -0.27, -0.66, and -0.84 V for NRR, respectively.