Rational design of graphdiyne-based single-atom catalysts for electrochemical CO_2 reduction reaction

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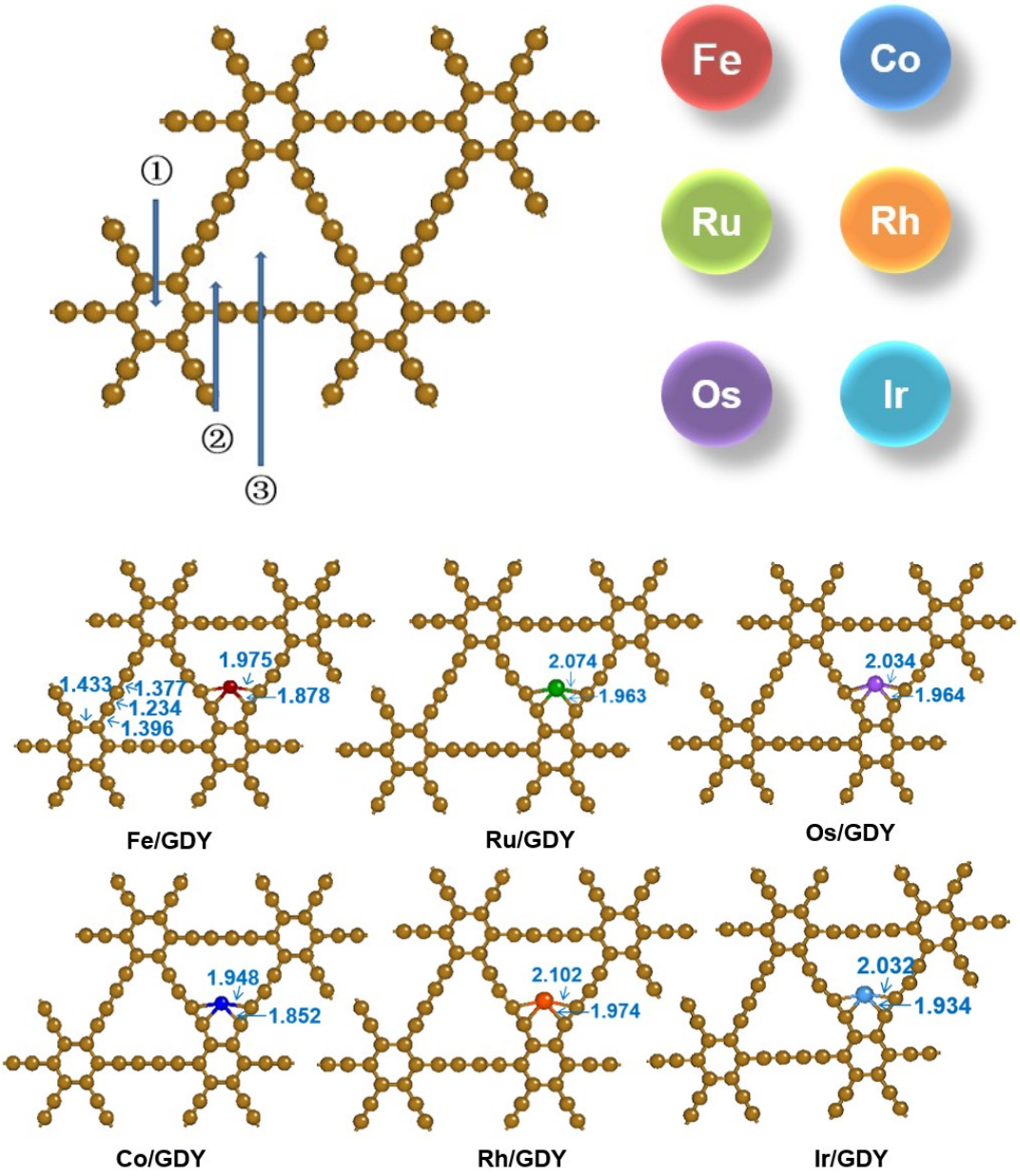

Figure S1. The optimized structure of TM_1/GDY and the schematic of screening site GDY.

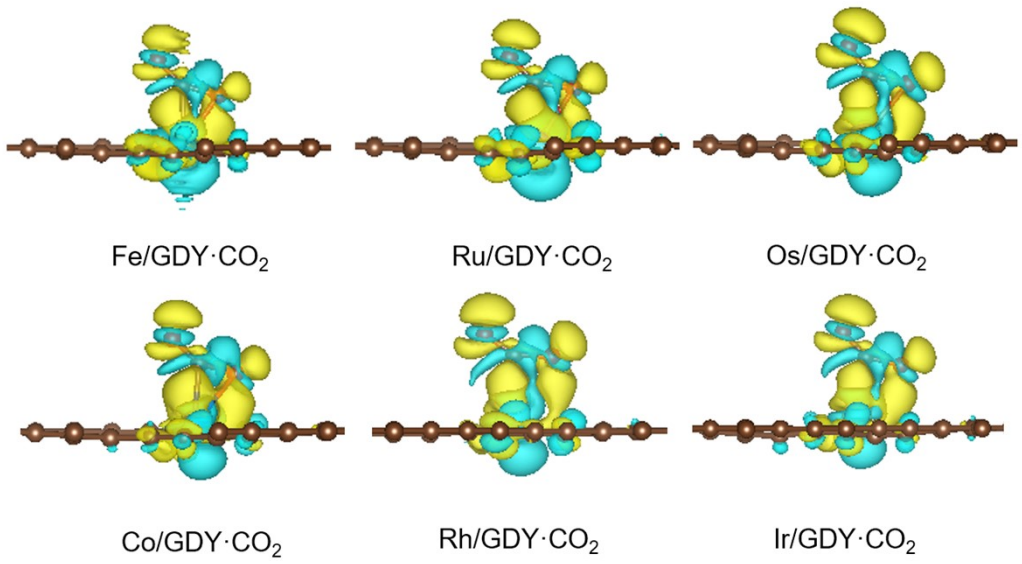

Figure S2. Differential charge density diagram of CO_2 adsorbed by TM_1/GDY.

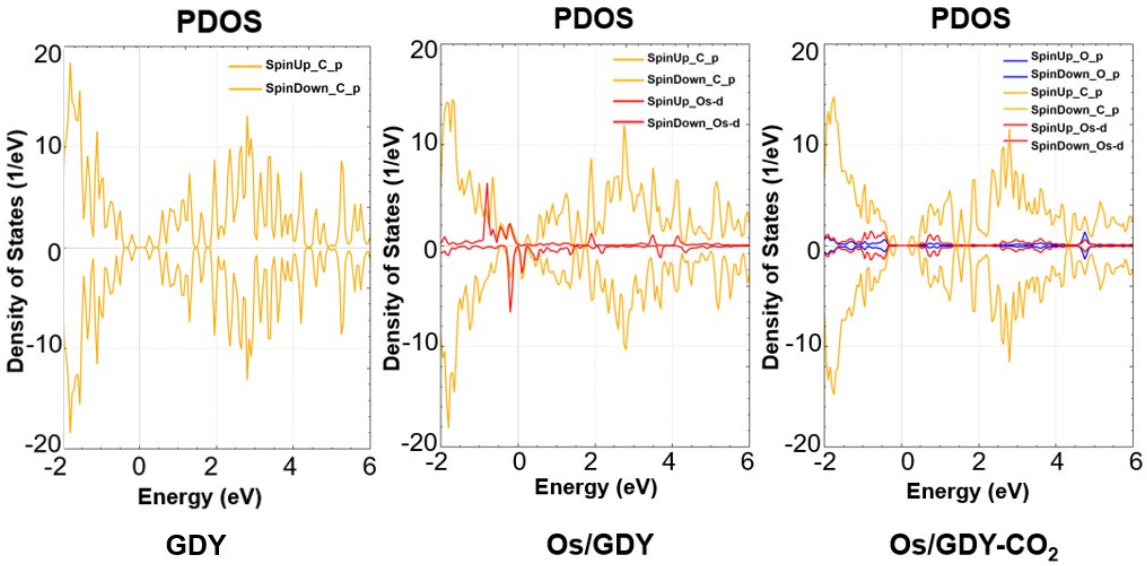

Figure S3. The schematic diagram of projected electronic densities of states of GDY, Os_1/GDY, and Os_1/GDY-CO_2.

Table S1 The change of free energy in the first protonation step of CO2RR adsorption and HER on TM_1/GDY catalysts.

SACs	ΔG_{HER} (eV)	ΔG_{CO2RR} (eV)
Fe/GDY	0.16	0.31
Ru/GDY	-0.95	-0.69
Os/GDY	-1.15	-0.51
Co/GDY	0.18	0.43
Rh/GDY	-0.31	0.39
Ir/GDY	-0.47	0.24

Table S2 The free energies of CO_2RR on Os/GDY.

CO_2RR	ΔG (eV)
$CO_2 \rightarrow *CO_2$	-0.52
$*CO_2 \rightarrow *COOH$	-0.57
$*COOH \rightarrow *CO$	-1.40
$*CO \rightarrow *COH$	-0.14
$*CO \rightarrow *CHO$	-0.79
$*CHO \rightarrow *CHOH$	-0.91
$*CHO \rightarrow *CH_2O$	-1.17
$*CH_2O \rightarrow *CH_2OH$	-1.03
$*CH_2O \rightarrow *CH_3O$	-1.66
$*CH_3O \rightarrow *CH_3OH$	-0.88
$*CH_3O \rightarrow *OCH_4$	-2.33
$*OCH_4 \rightarrow CH_4$	-2.12