

Electrocatalytic Oxygen Reduction to Hydrogen Peroxide on Graphdiyne-Based Single-Atom Catalysts: First-Principles Studies

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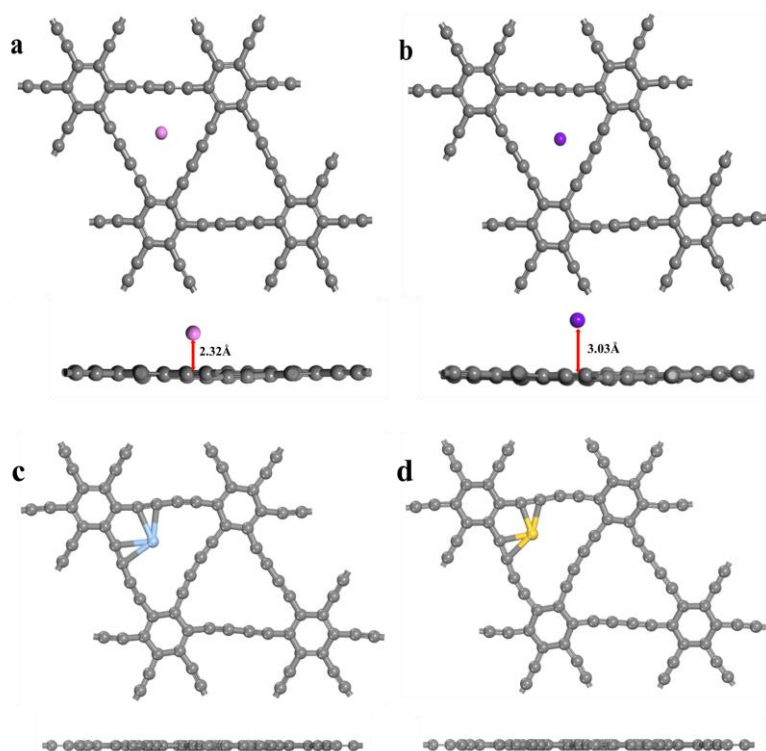


Figure S1. Top and side views of the (a) Zn atom, (b) Cd atom, (c) Ag atom and (d) Au atom supported on GDY. Color scheme: C: Gray; Zn: Pink; Cd: Purple; Ag: Blue; Au: Yellow.

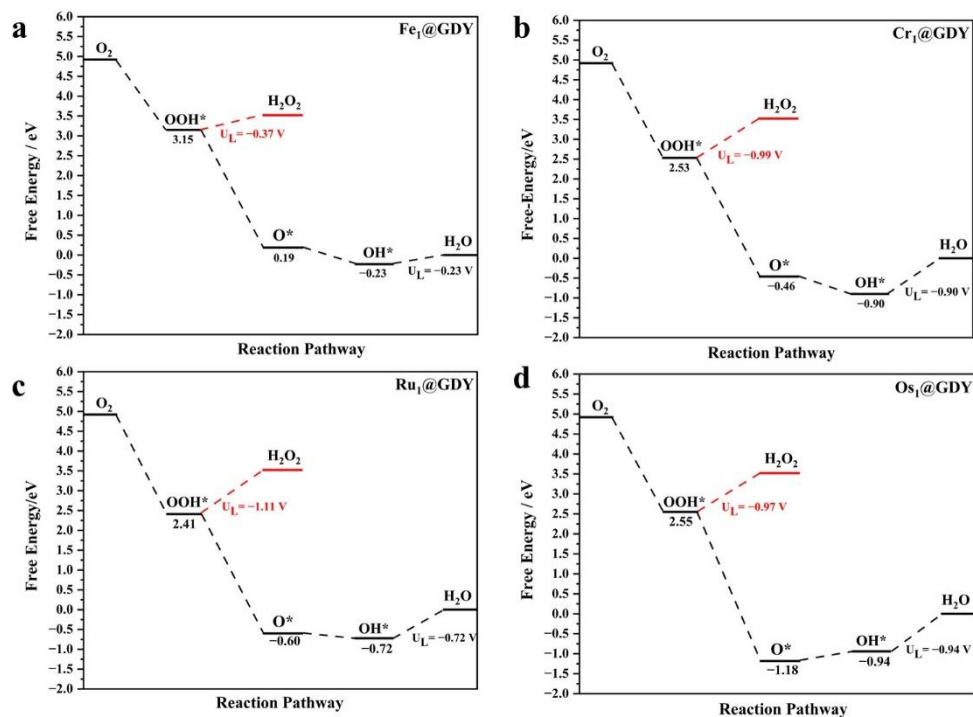


Figure S2. Free energy diagrams of 2e⁻ and 4e⁻ ORR on (a): Fe₁@GDY; (b): Cr₁@GDY; (c): Ru₁@GDY; d: Os₁@GDY.

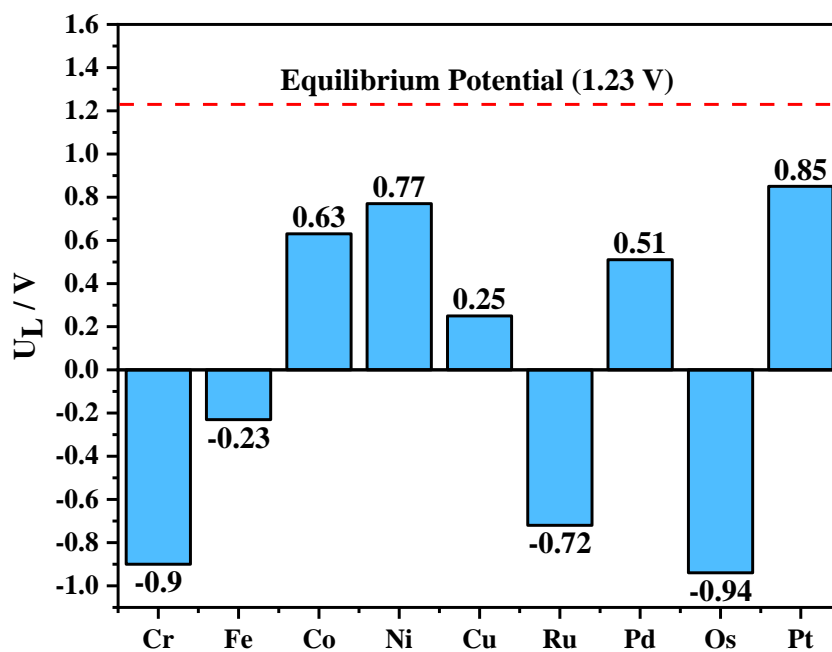


Figure S3. Limiting potentials of 4e⁻ ORR on TM₁@GDY (TM=Cr, Fe, Co, Ni, Cu, Ru, Pd, Os, and Pt) catalysts. The red line represents the equilibrium potential of 4e⁻ ORR.

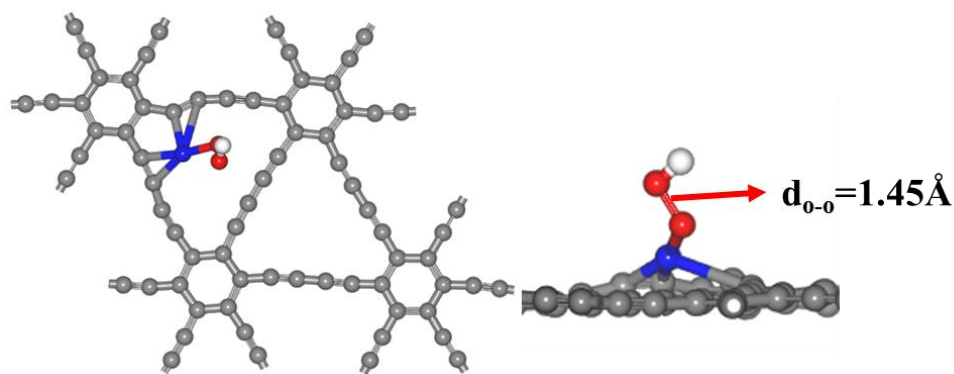


Figure S4. The adsorption structure of OOH* on Pt₁@GDY and the O–O bond length.

Table S1. The E_b on TM₁@GDY.

TM ₁ @GDY	E _b (eV)
Sc ₁ @GDY	–4.41
Ti ₁ @GDY	–4.57
V ₁ @GDY	–3.54
Cr ₁ @GDY	–3.62
Mn ₁ @GDY	–2.39
Fe ₁ @GDY	–3.39
Co ₁ @GDY	–4.08
Ni ₁ @GDY	–4.26
Cu ₁ @GDY	–2.00
Zn ₁ @GDY	–0.19
Y ₁ @GDY	–4.67
Zr ₁ @GDY	–5.54
Nb ₁ @GDY	–5.58
Mo ₁ @GDY	–2.96
Ru ₁ @GDY	–4.65
Rh ₁ @GDY	–4.01

Pd ₁ @GDY	-2.68
Ag ₁ @GDY	-0.71
Cd ₁ @GDY	-0.19
Hf ₁ @GDY	-5.20
Ta ₁ @GDY	-5.15
W ₁ @GDY	-3.87
Re ₁ @GDY	-3.28
Os ₁ @GDY	-5.13
Ir ₁ @GDY	-4.89
Pt ₁ @GDY	-4.06
Au ₁ @GDY	-0.85

Table S2. The G_{OOH}* on TM₁@GDY.

TM ₁ @GDY	G _{OOH} * (eV)
Sc ₁ @GDY	2.07
Ti ₁ @GDY	1.61
V ₁ @GDY	1.63
Cr ₁ @GDY	2.53
Mn ₁ @GDY	2.95
Fe ₁ @GDY	3.15
Co ₁ @GDY	3.44
Ni ₁ @GDY	3.76
Cu ₁ @GDY	3.50
Y ₁ @GDY	2.17
Zr ₁ @GDY	1.37
Ru ₁ @GDY	2.41
Rh ₁ @GDY	3.17
Pd ₁ @GDY	4.41

Hf@GDY	1.57
Os@GDY	2.55
Ir@GDY	2.94
Pt@GDY	4.07