

Supporting information

Single Layer of Polymeric Metal-phthalocyanine: Promising Substrate to Realize
Single Pt Atom Catalyst with Uniform Distribution

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Table S1. Geometrical parameters (Å) for Pt/TMPcs, mulliken analysis of the charges and magnetic moments for Pt atoms in Pt/TMPcs.

TM-Pc	E_{ad} (eV)	d_{Pt-M}	d_{Pt-N}	$M_{\mu B}$	C_{Pt}
Sc		2.49	3.88	0.97	-0.34
Ti		2.18	3.46	0	-0.37
V		2.16	3.35	-0.18	-0.27
Cr		2.15	3.25	0	-0.18
Mn		2.27	3.17	0.76	-0.10
Fe		2.26	3.13	0.77	-0.06
Co		2.44	3.18	0.98	-0.03
Ni		2.61	3.32	0.34	-0.20
Cu		2.64	3.36	1.82	-0.03
Zn		2.54	3.71	1.50	-0.13

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Figure S1. Schematic energy profile and corresponding local configurations of CO molecule directly react with adsorbed O₂ molecule. All energies are given with respect to the reference energy.

