Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Oxygen reduction reaction on cobalt−(*n*)pyrrole clusters from DFT studies

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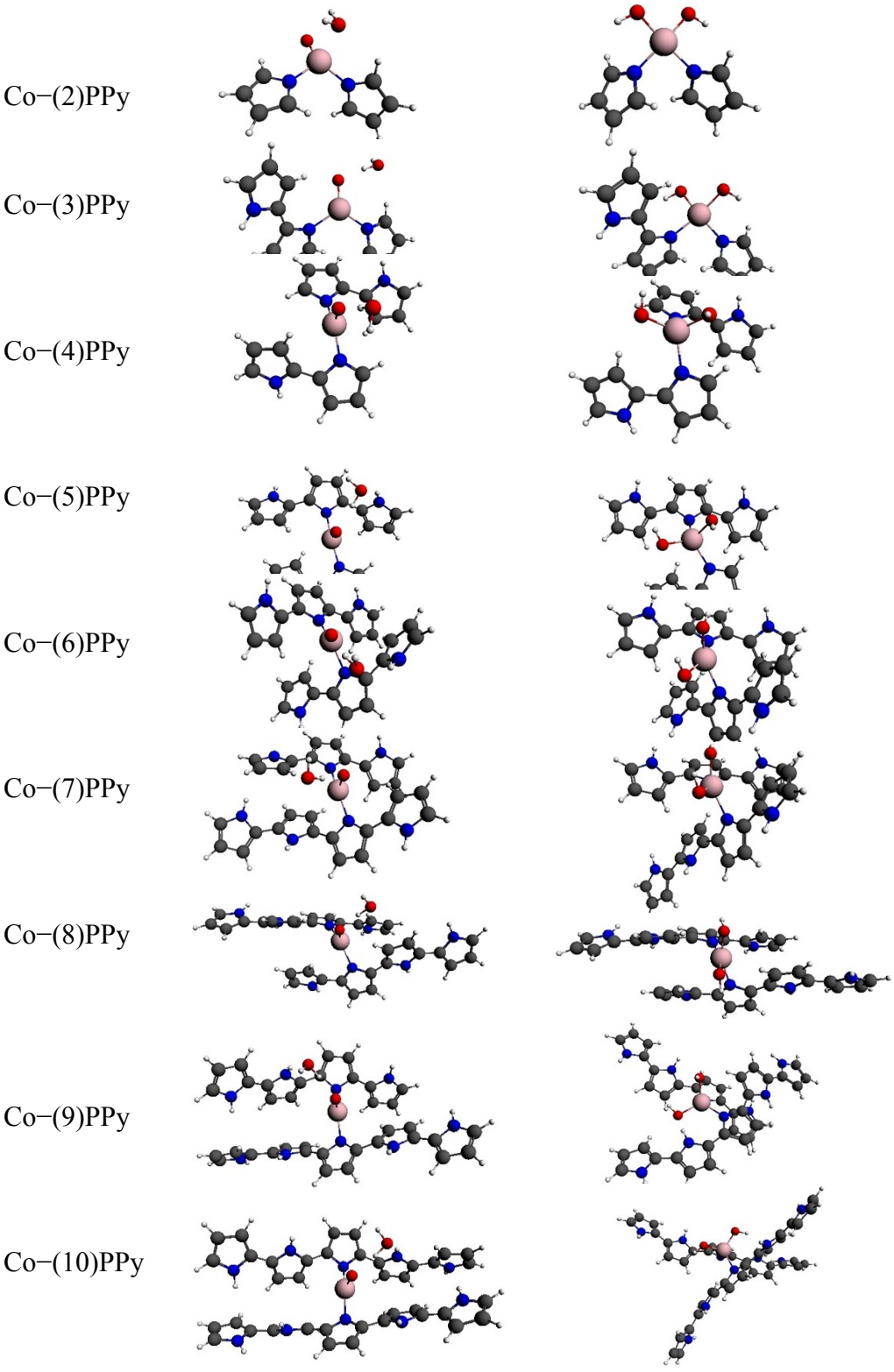

Fig. S1 Optimized structures of Co−(*n*)PPy−H_2O−O and Co−(*n*)PPy−HO−OH.

Table S1 Calculated key bond lengths, R (Å), and bond angels, θ (deg), for the Co−(*n*)PPy−H_2O−O complexes (the data corresponding to the Co−(*n*)PPy−HO−OH are given in

the parentheses)

Co−(*n*)PPy	$R_{Co(1)-N(2)}$	$R_{Co(1)-N(3)}$	$R_{Co(1)-O(4)}$	$R_{Co(1)-O(5)}$	$R_{O(5)-O(6)}$	$\theta_{N(2)Co(1)N(3)}$
Co−(2)PPy	1.915	1.875	1.668	2.288	2.809	102.4
	(1.984)	(1.985)	(1.821)	(1.822)	(2.509)	(89.1)
Co−(3)PPy	2.062	1.976	1.703	3.821	2.821	110.8
	(2.005)	(1.952)	(1.821)	(1.832)	(2.552)	(91.9)
Co−(4)PPy	1.929	1.925	1.65	4.344	2.895	145.5
	(2.059)	(2.044)	(1.882)	(1.894)	(3.081)	(116.3)
Co−(5)PPy	1.944	1.931	1.66	3.976	2.924	146.5
	(2.133)	(2.029)	(1.871)	(1.894)	(3.099)	(117)
Co−(6)PPy	2.053	2.081	1.708	4.038	2.741	118.3
	(2.032)	(2.035)	(1.818)	(1.827)	(2.557)	(102.8)
Co−(7)PPy	1.96	1.972	1.654	3.94	2.852	153.7
	(2.025)	(2.055)	(1.816)	(1.826)	(2.549)	(102.3)
Co−(8)PPy	2.051	2.059	1.718	4.122	2.779	124.9
	(2.011)	(2.015)	(1.836)	(1.84)	(2.564)	(96.1)
Co−(9)PPy	1.954	1.957	1.655	4.144	2.816	151.4
	(2.098)	(2.12)	(1.896)	(1.958)	(3.127)	(113.2)
Co−(10)PPy	1.982	1.945	1.658	4.028	2.845	154
	(2.121)	(2.14)	(1.858)	(1.859)	(2.991)	(112.7)