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Supplementary Information

The Potential of Zero Charge and Solvation Effects on Single-Atom M–N–C Catalysts for Oxygen Electrocatalysis

Di Zhang* and Hao Li*

Advanced Institute for Materials Research (WPI-AIMR), Tohoku University, Sendai 980-8577, Japan

*** Corresponding Authors:**

di.zhang.a8@tohoku.ac.jp (D. Z.)

li.hao.b8@tohoku.ac.jp (H. L.)

Table S1 Comparison between the potential of zero charges (PZCs) acquired from explicit and implicit solvation models (unit: V/SHE)

M-N-C catalysts	Explicit solvation PZCs	Implicit solvation PZCs
Cr-pyrrole-N_4	0.054 ± 0.03	-0.150
Mn-pyrrole-N_4	0.254 ± 0.05	-0.056
Fe-pyrrole-N_4	0.338 ± 0.04	0.055
Co-pyrrole-N_4	0.384 ± 0.07	0.119
Ni-pyrrole-N_4	0.354 ± 0.07	0.205
Cu-pyrrole-N_4	0.428 ± 0.08	0.174
Cr-pyridine-N_4	-0.864 ± 0.05	-0.897
Mn-pyridine-N_4	-0.787 ± 0.02	-0.679
Fe-pyridine-N_4	-0.618 ± 0.05	-0.665
Co-pyridine-N_4	-0.526 ± 0.06	-0.611
Ni-pyridine-N_4	-0.335 ± 0.03	-0.575
Cu-pyridine-N_4	-0.506 ± 0.05	-0.644

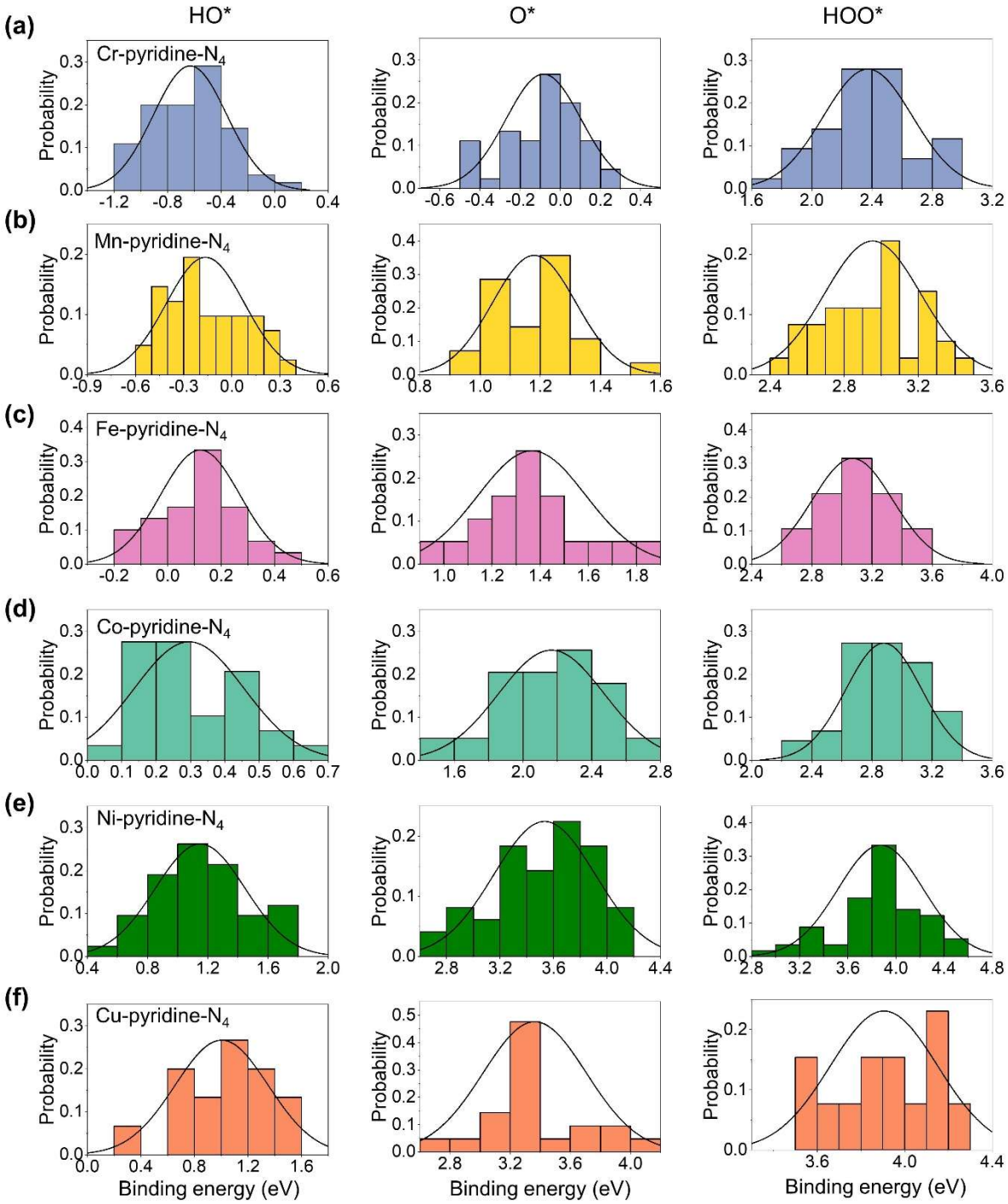

Figure S1. Solvation effects on the adsorption energies of HO*, O*, and HOO* on M-N-C Catalysts. Panels (**a-f**) detail the adsorption energies of HO*, O*, and HOO* in a solvation environment on (**a**) Cr-, (**b**) Mn-, (**c**) Fe-, (**d**) Co-, (e) Ni-, and (**f**) Cu-pyridine-N, respectively.

Table S2 Summary of the implicit solvation effects (E_{ads*}^{change}) on M-N-C catalysts calculated based on the VASPsol package. (Unit: eV)

Metal site	M_1-pyrrole-N_4			M_1-pyridine-N_4		
	HO*	**O***	**HOO***	**HO***	**O***	**HOO***
Cr	-0.188	-0.018	-0.225	-0.157	-0.059	-0.325
Mn	-0.034	-0.226	-0.080	-0.172	0.031	-0.671
Fe	0.033	-0.055	-0.138	-0.153	-0.208	-0.234
Co	-0.371	-0.067	-0.427	-0.169	-0.090	-0.548
Ni	-0.250	-0.073	-0.072	-0.289	-0.258	-0.235
Cu	-0.337	-0.667	-0.203	-0.150	-0.500	-0.713

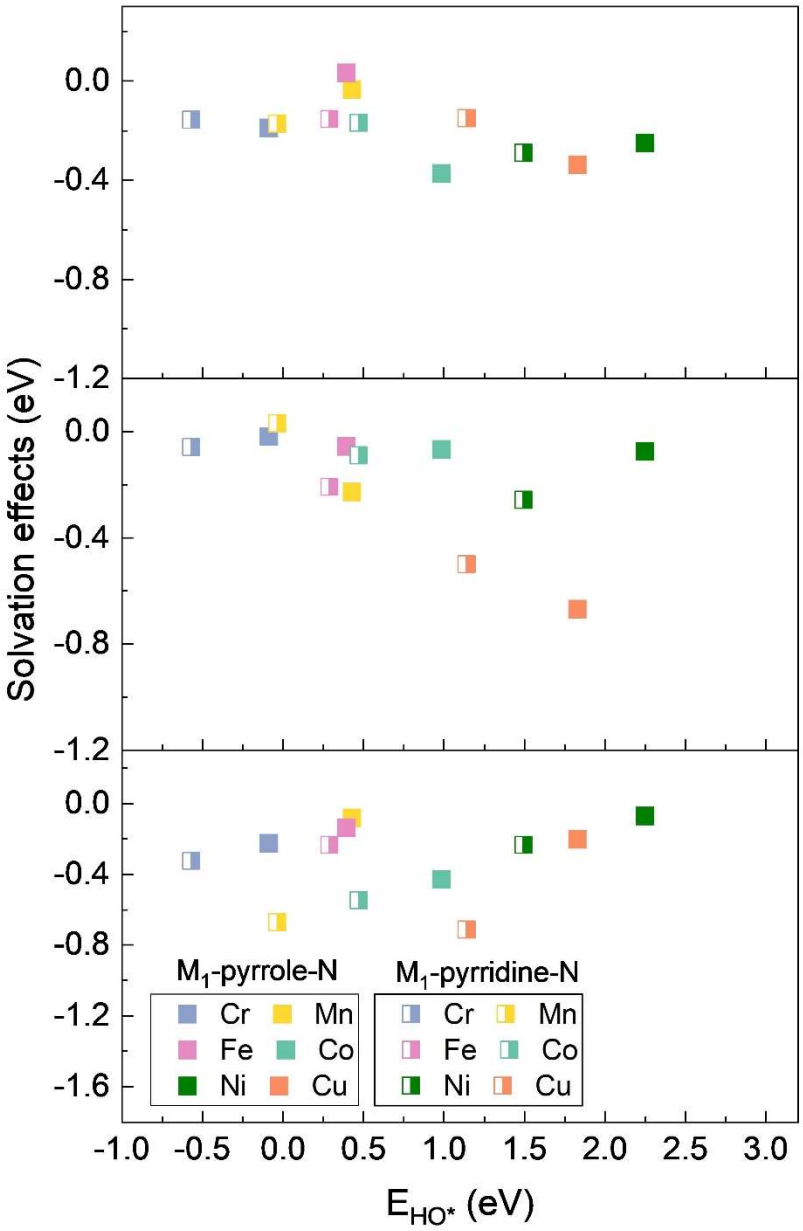

Figure S2. Analyses of implicit solvation effects on the adsorption energies of HO*, O*, and HOO*.