

Engineering Zeolitic Imidazolate Framework Derived Mo-Doped Cobalt Phosphide for Efficient OER Catalysts

Mohammad Atiqur Rahman,^{a,b,c} Ze Cai,^a Zannatul Mumtarin Moushumi,^d Ryuta Tagawa,^a Yoshiharu Hidaka,^a Chiyu Nakano,^e Md. Saidul Islam,^{a,f} Yoshihiro Sekine,^{a,g} Yuta Nishina,^e Shintaro Ida,^f and Shinya Hayami^{,a,f,h}*

^a. Department of Chemistry, Graduate School of Science and Technology, Kumamoto University, 2-39-1 Kurokami, Chuo-ku, Kumamoto 860-8555, Japan

^b. Department of Chemistry, Comilla University, Cumilla-3500, Bangladesh

^c. International Research Organization for Advanced Science and Technology, Kumamoto University, 2-39-1 Kurokami, Chuo-ku, Kumamoto 860-8555, Japan

^d. Department of Applied Chemistry and Biochemistry, Graduate School of Science and Technology, Kumamoto University, 2-39-1 Kurokami, Chuo-ku, Kumamoto 860-8555, Japan

^e. Research Core for Interdisciplinary Sciences, Okayama University Professor (Research), Graduate School of Natural Science and Technology, Okayama University

^f. Institute of Industrial Nanomaterials (IINa), Kumamoto University, 2-39-1 Kurokami, Chuo-ku, Kumamoto 860-8555, Japan.

^g. Priority Organization for Innovation and Excellence, Kumamoto University, 2-39-1 Kurokami, Chuo-ku, Kumamoto 860-8555, Japan.

^h. International Research Center for Agricultural and Environmental Biology (IRCAEB), 2-39-1

Kurokami, Chuo-ku, Kumamoto 860-8555, Japan.

*Corresponding author

Email: hayami@kumamoto-u.ac.jp

Table S1: Microstructural parameters of CoP and CoMoP-2 Catalysts

Catalysts	2 Θ value	Plane	a=b=c (Å)	d-spacing	Average Crystalline size (nm)
CoP	49.01	202	5.050	1.86	8.34
CoMoP-2	48.33	202	5.077	1.88	4.58

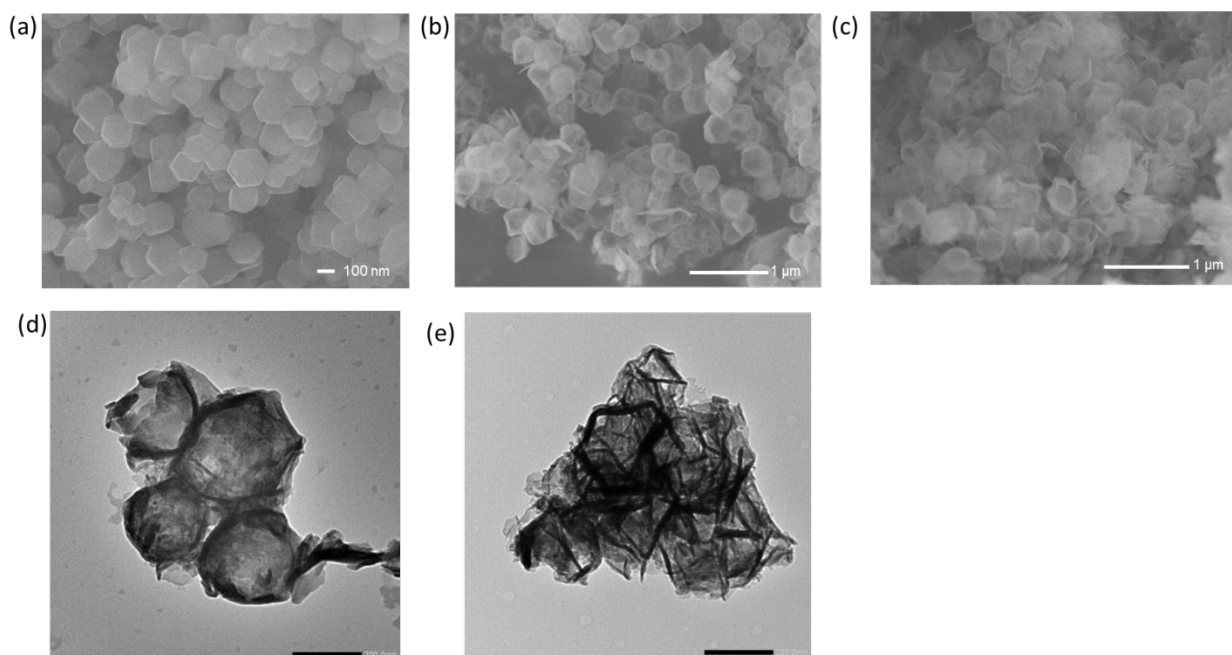


Figure S1: SEM images of: (a) ZIF-67, (b) CoMoP-1, (c) CoMoP-3, and TEM images of (d) CoMoP-1, and (e) CoMoP-3.

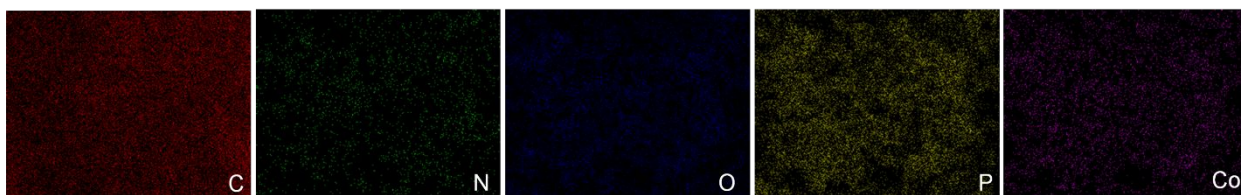
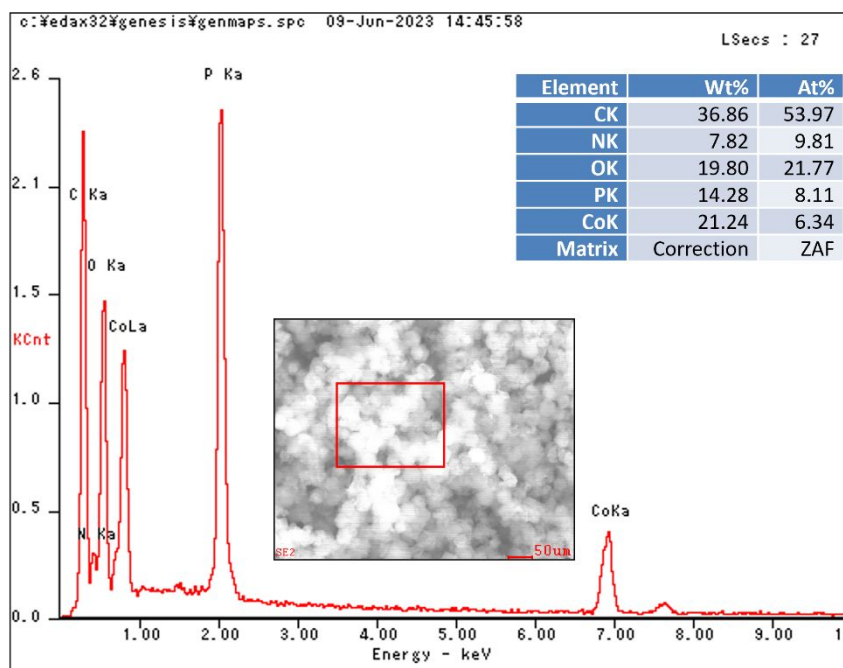


Figure S2: EDX analysis of ZIF-67 derived CoP.

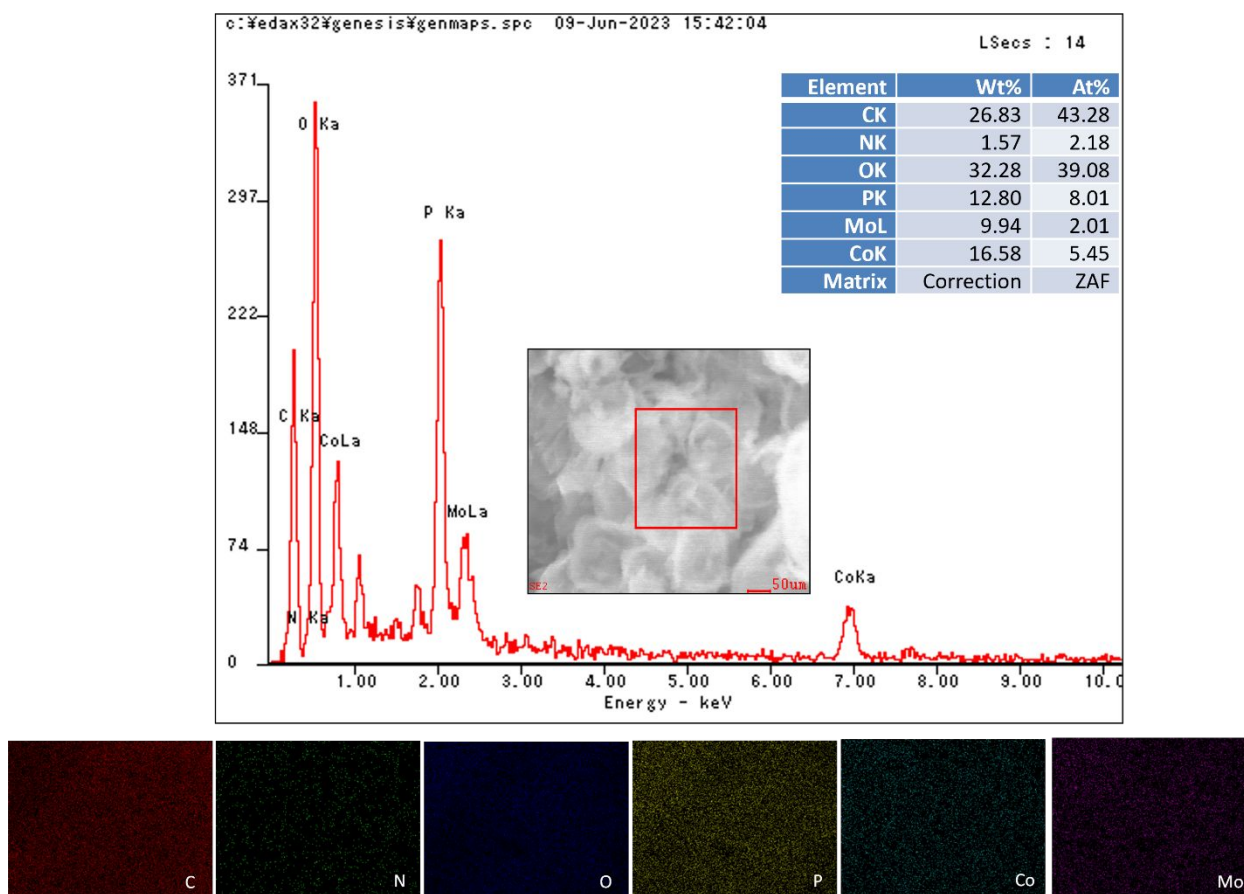


Figure S3. EDX analysis of ZIF-67 derived CoMoP-2.

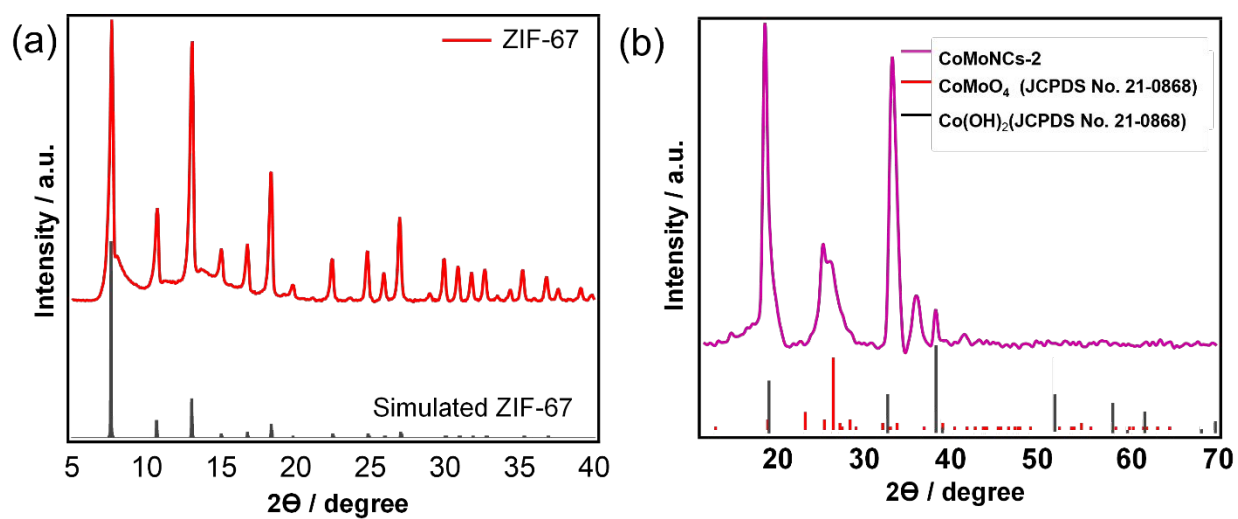


Figure S4: PXRD pattern of: (a) ZIF-67, and (b) CoMoNCs-2.

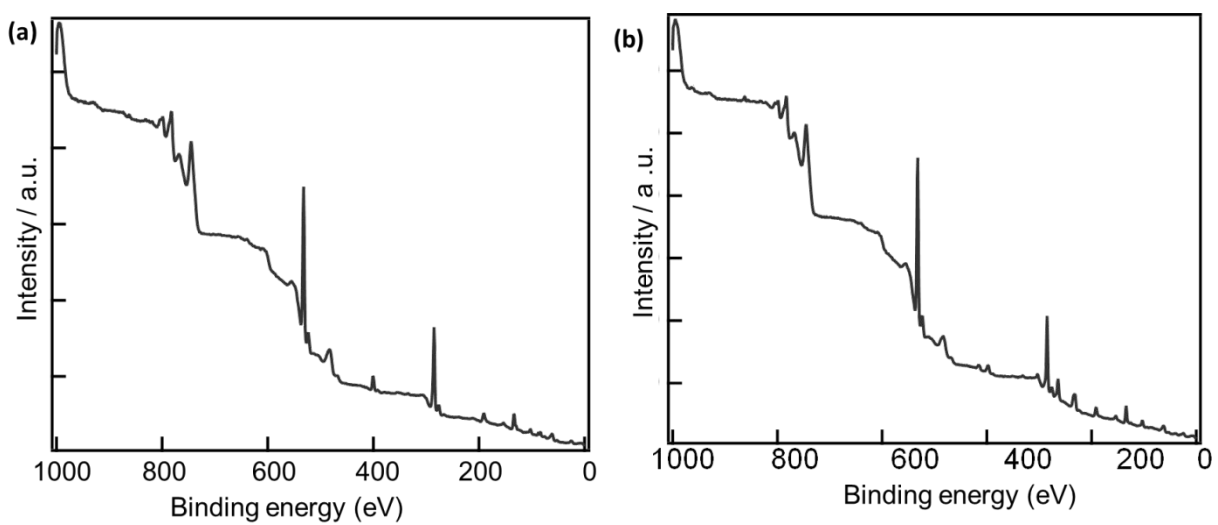


Figure S5: XPS Survey spectrum of: (a) CoP, and (b) CoMoP-2.

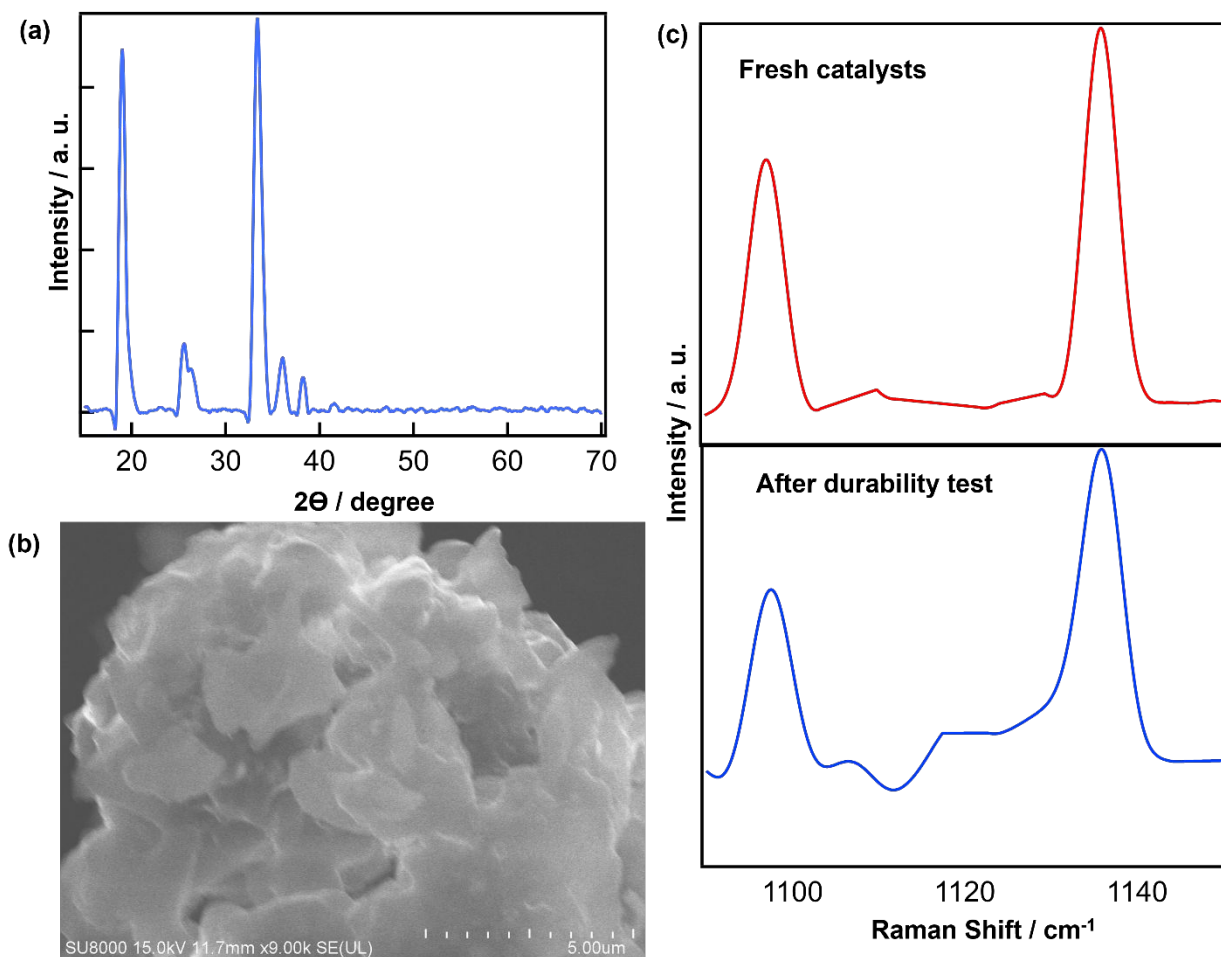


Figure S6: (a) PXRD pattern, (b) FESEM image, and (c) Raman shift of CoMoP-2 catalysts before and after durability test at 10 mA cm^{-2} for 4h.

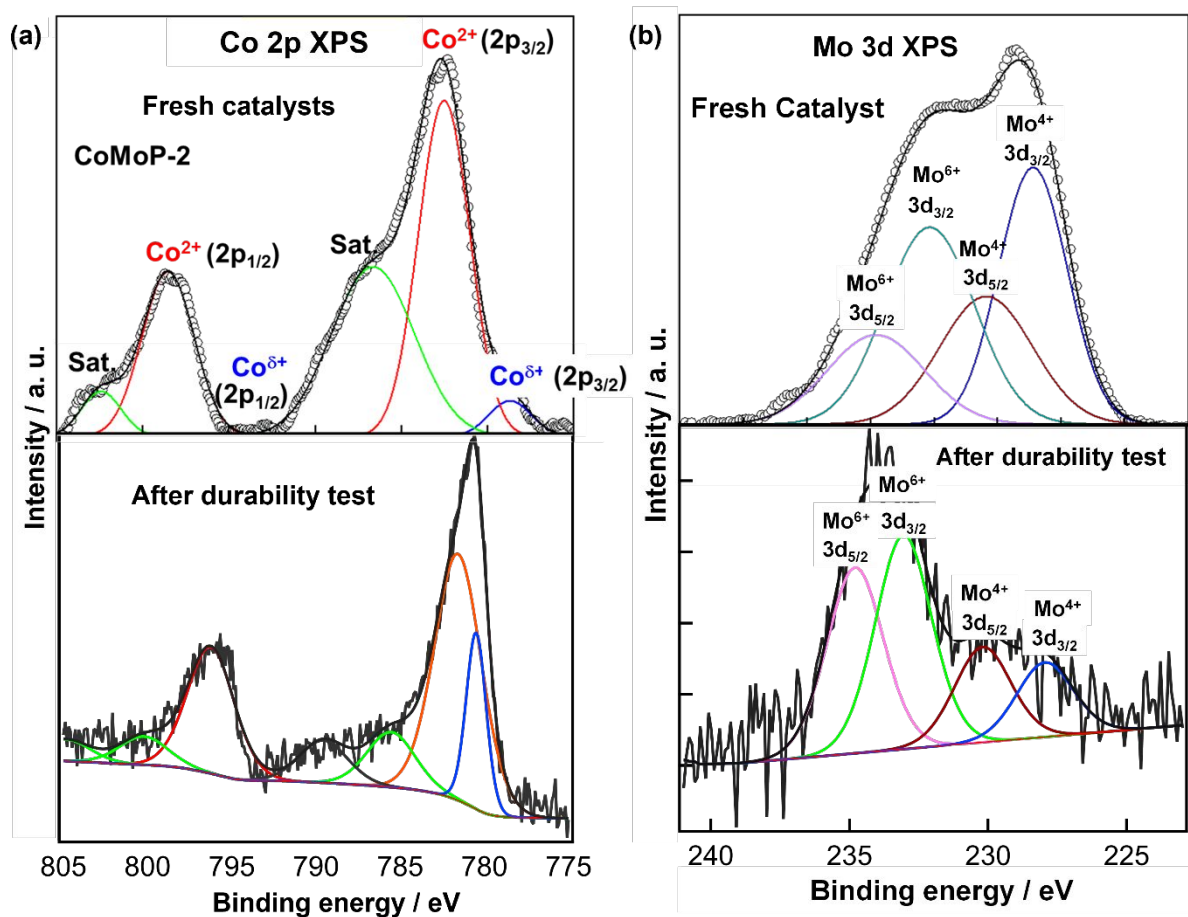


Figure S7: XPS of spectrum: (a) Co 2p, and (b) Mo 3d of CoMoP-2 catalysts before and after durability test at 10 mA cm⁻² for 4h.

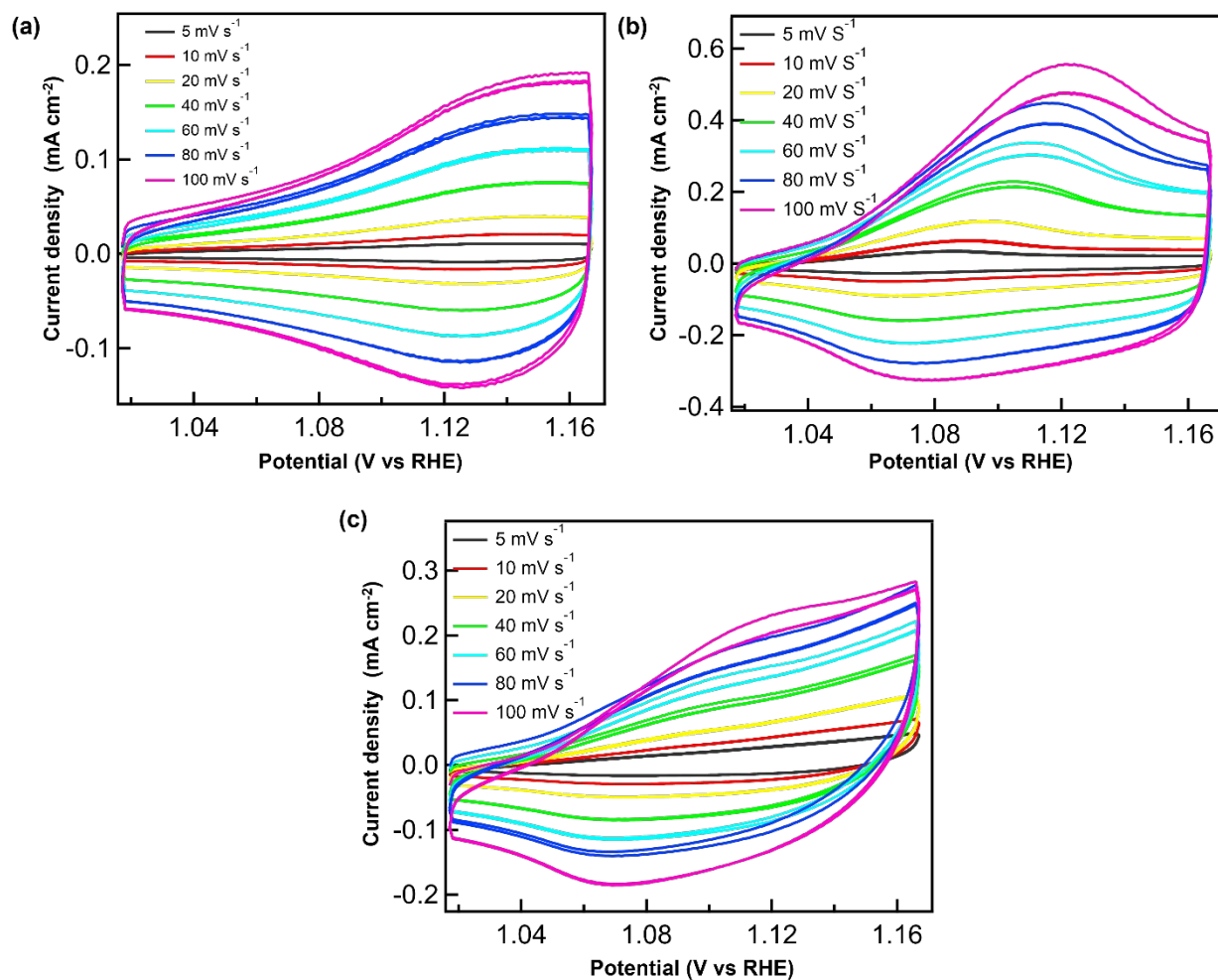


Figure S8: CV curves at various scan rates ranging from 5 to 100 mV s⁻¹ of: (a) CoP, (b) CoMoP-1, and (c) CoMoP-3 each of which was measured at different scan rate in 1.0 M KOH solution.

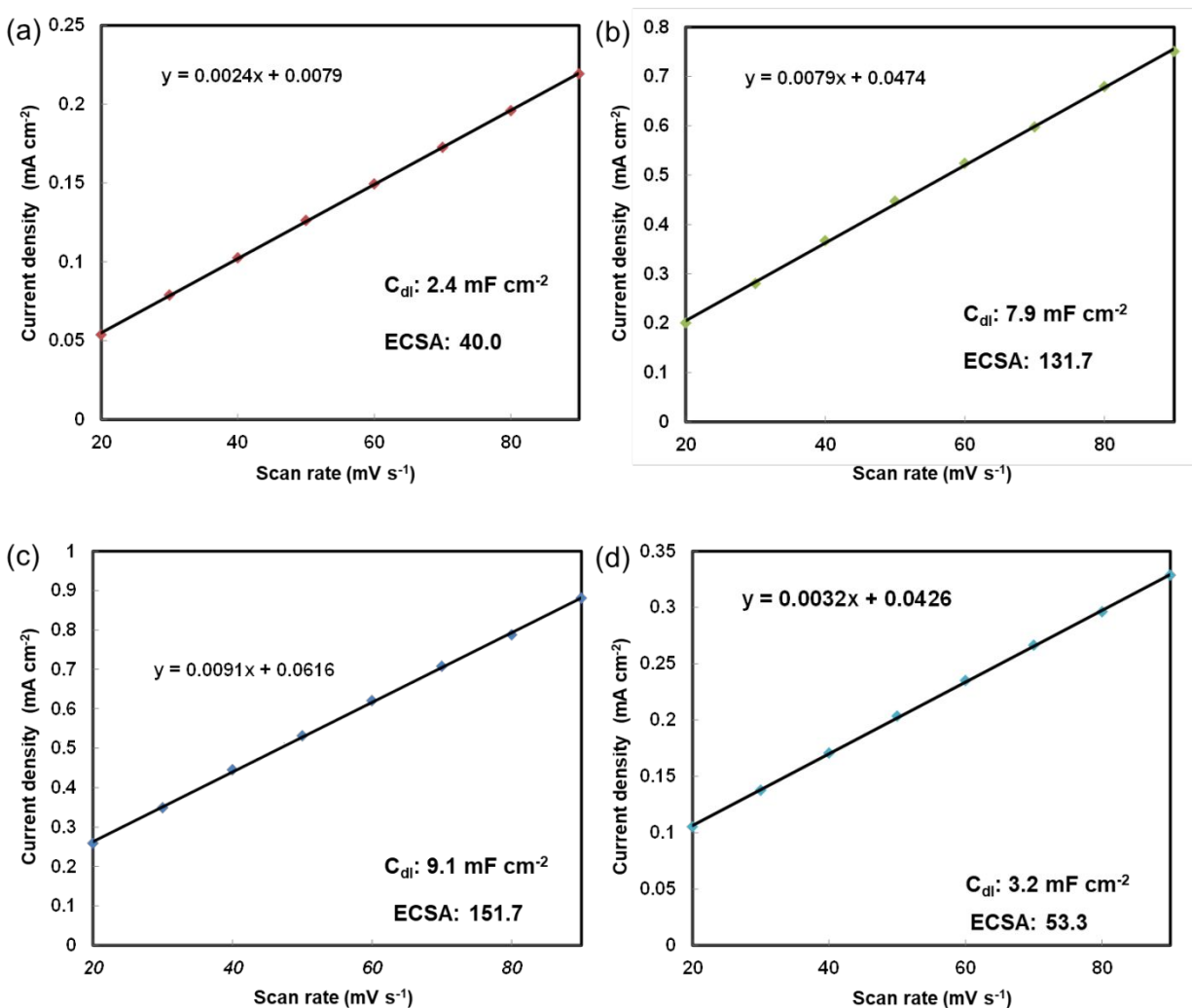


Figure S9: Current density vs Scan rate, calculated C_{dl} values and ECSA values of (a) CoP, (b) CoMoP-1, (c) CoMoP-2, and (d) CoMoP-3 obtained from the CV curves measured at various scan rates.

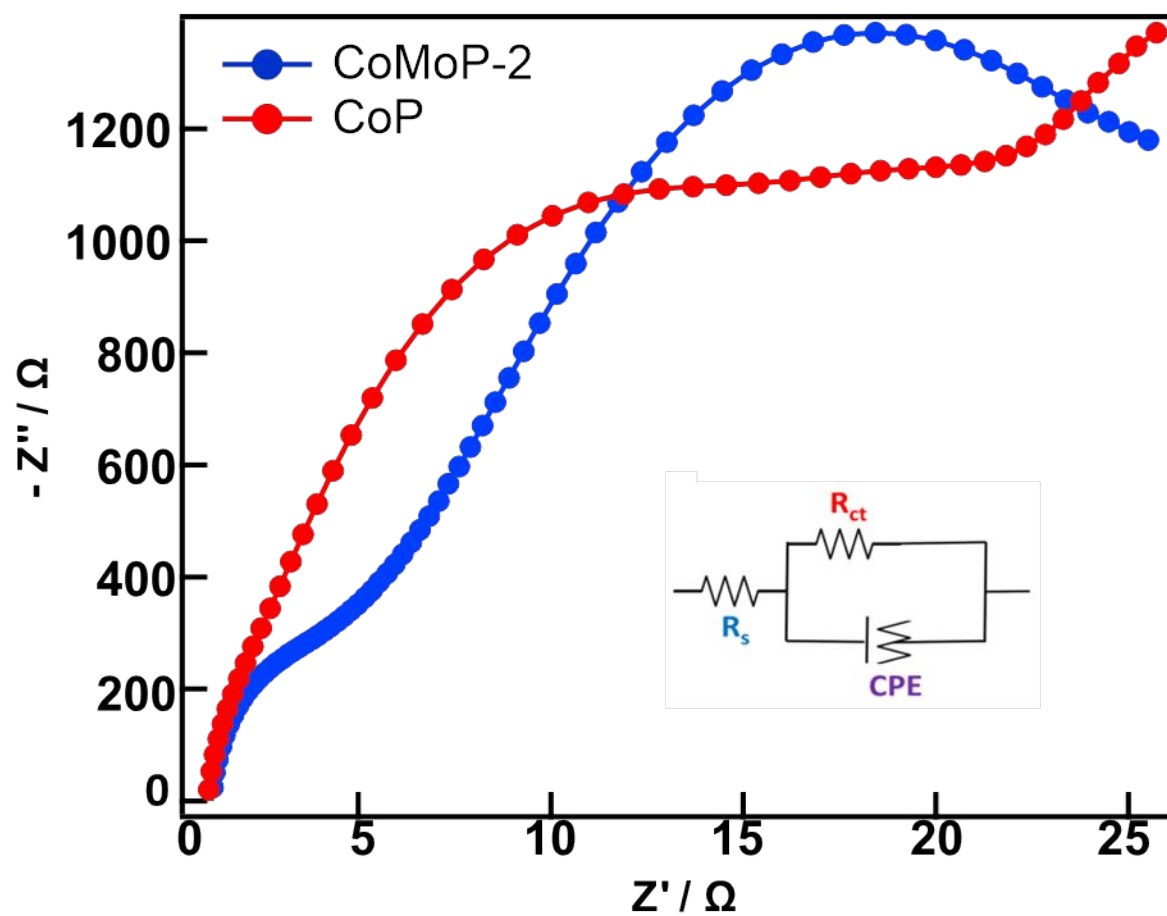


Figure 10: Nyquist plots of CoP and CoMoP-2 catalysts measured in 1.0 M KOH solution.

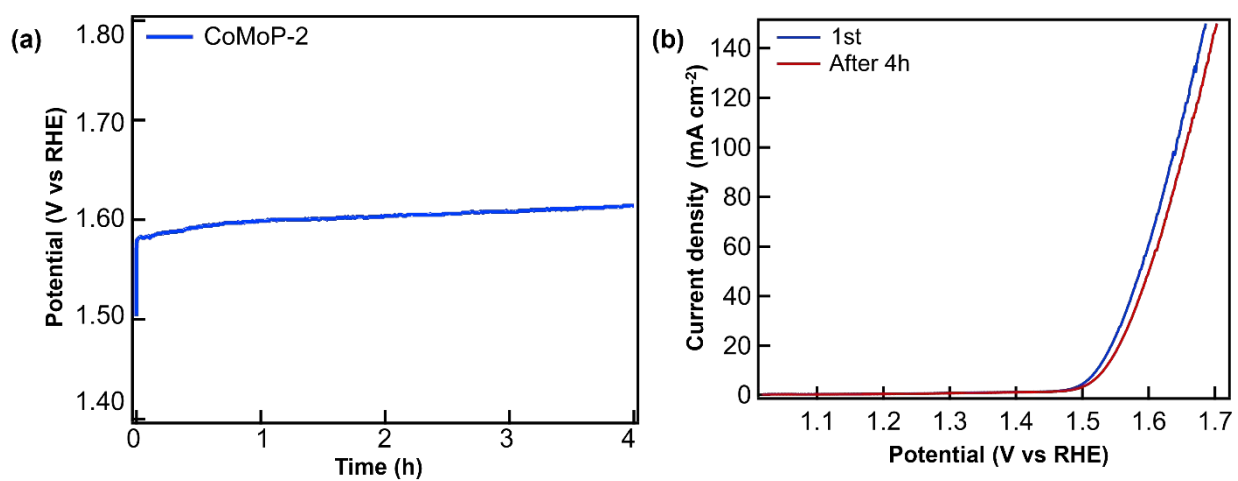


Figure S11: (a) Stability test of CoMoP-2 Chronoamperometry study, (b) LSV curves before and after the stability test.

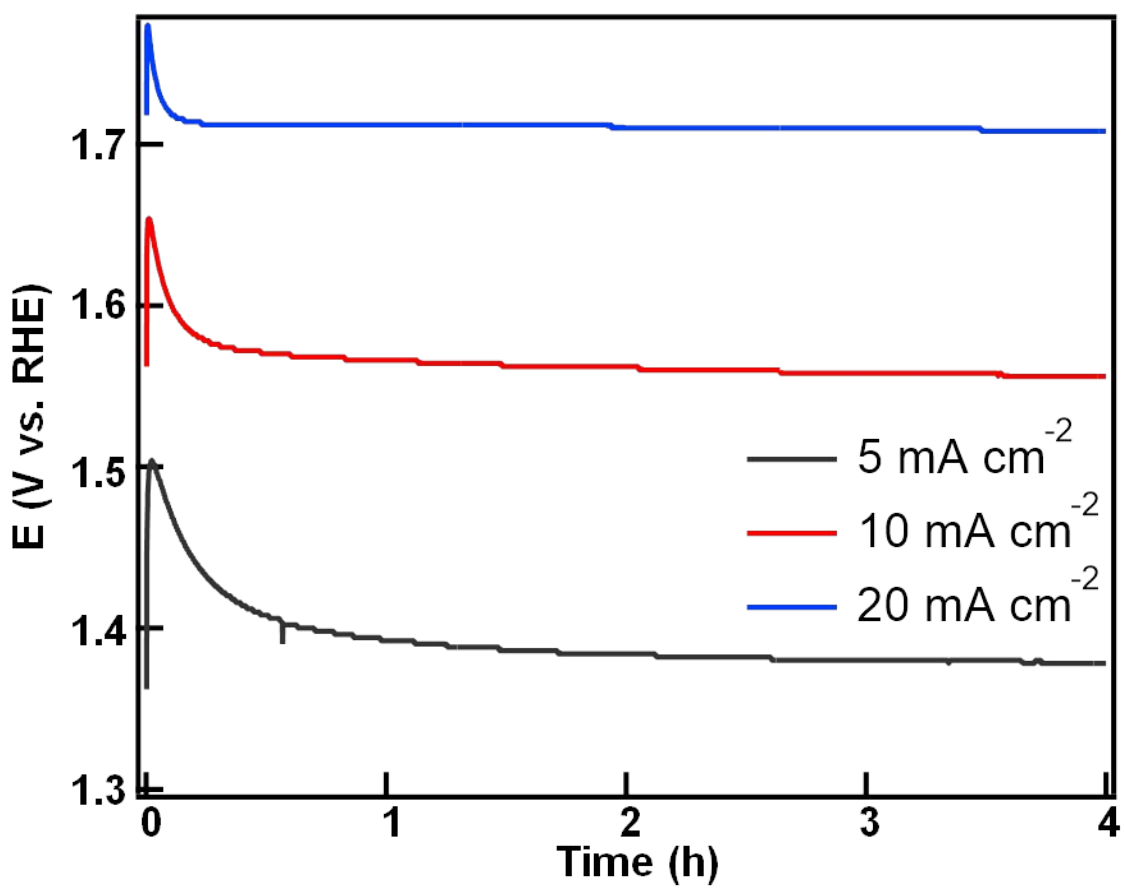


Figure S12: Stability test of CoMoP-2 Chronopotentiometry study at various current densities for 4 h.