Supplementary Information (SI) for New Journal of Chemistry. This journal is © The Royal Society of Chemistry and the Centre National de la Recherche Scientifique 2024

Electronic Supporting Information

Supramolecular and Electrocatalytic OER properties of new heteroleptic fluoro- and trifluoromethyl- substituted Ni(II)-dithiolates: Effect of substituents and dihedral angle on electrocatalytic performance

Aparna Kushwaha,^a Devyani Srivastava,^a Gabriele Kociok-Köhn,^b Suresh W. Gosawi,^c Ratna Chauhan,^d Sarfaraz Ahmed,^e Abhinav Kumar,^a*

^aDepartment of Chemistry, Faculty of Science, University of Lucknow, Lucknow 226 007, India. Email: abhinavmarshal@gmail.com

^bPhysical Structures Characterisation, University of Bath, Claverton Down, Bath, BA2 7AY, UK.

^cDepartment of Physics, Savitribai Phule Pune University, Pune-411007, India.

^dDepartment of Environmental Science, Savitribai Phule Pune University, Pune-411007, India.

^eDepartment of Pharmacognosy, College of Pharmacy, King Saud University, P.O. Box 2457 Riyadh 11451, Saudi Arabia



Fig. S1 Linear Sweep Voltammograms of (a)-(d) of Ni-1, Ni-2, Ni-3 and Ni-4, respectively at 10, 20, 50 and 100 mV/s scan rates.



Fig S2. Cyclic voltammogram for (a) **Ni-1**, (b) **Ni-2**, (c) **Ni-3** and (d) **Ni-4** in 0.1 M KOH at different scan rates; plots constructed between current density and scan rates (e) **Ni-1**, (f) **Ni-2**, (g) **Ni-3** and (h) **Ni-4**.



Fig. S3 Chronoamperometry plots (a)-(d) of Ni-1, Ni-2, Ni-3 and Ni-4, respectively; Chronopotentiometry plots (e)-(h) of Ni-1, Ni-2, Ni-3 and Ni-4, respectively.

Electronic Supporting Information



Fig. S4 FESEM images for (a) and (e) **Ni-1**; (b) and (f) **Ni-2**; (c) and (g) **Ni-3**; (d) and (h) **Ni-4** before and after OER electrocatalysis.