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Supporting information

Probing the activity and stability of MoO_2 surface nanorod arrays for hydrogen evolution in an anion exchange membrane multi-cell water electrolysis stack

Francesco Bartoli,[1,2] Marcello Marelli,[3] Claudio Evangelisti,[4] Laura Capozzoli,[1] Karel Bouzek,[5] Jaromir Hnát,[5] Giulia Serrano,[6] Lorenzo Poggini [1], Kevin Stojanovski,[7] Valentín Briega-Martos,[7] Serhiy Cherevko,[7] Hamish A. Miller,[1] Francesco Vizza[1]

[1] Institute of Chemistry of Organometallic Compounds – National Research Council of Italy (ICCOM-CNR), Via Madonna del Piano 10, 50019 Sesto Fiorentino (Florence), Italy.

[2] Department of Biotechnology, Chemistry and Pharmacy, University of Siena, Via Aldo Moro 2, 53100 Siena, Italy.

[3] Istituto di Scienze e Tecnologie Chimiche "Giulio Natta", CNR-SCITEC, 20138 Milano, Italy.

[4] Institute of Chemistry of Organometallic Compounds, ICCOM-CNR, 56124 Pisa, Italy.

[5] University of Chemistry and Technology, Prague, Department of Inorganic Technology, Technická 5, 166 28, Prague 6, Czech Republic.

[6] Department of Industrial Engineering (DIEF) and INSTM Research Unit, University of Florence, Via Santa Marta 3, 50139 Florence, Italy.

[7] Forschungszentrum Jülich GmbH, Helmholtz Institute Erlangen-Nürnberg for Renewable Energy (IEK-11), Cauerstr. 1, 91058 Erlangen, Germany

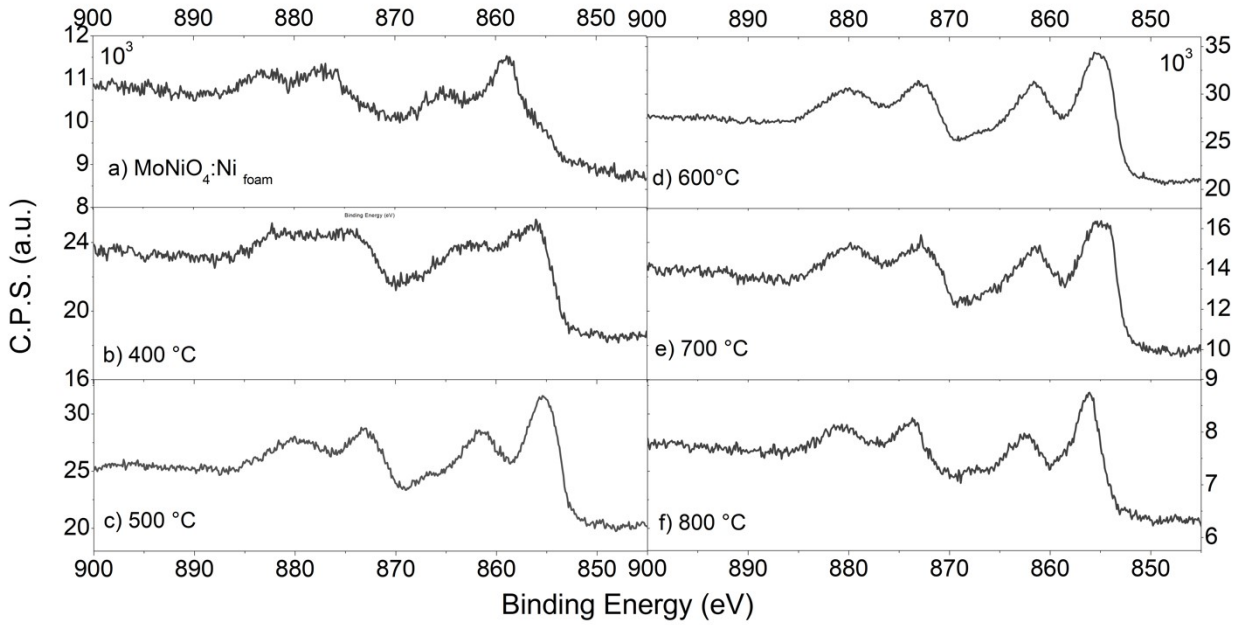


Figure S1: Ni 2p XPS of precursor $MoNiO_4$/Ni a) and MoO_2/Ni samples prepared at various temperatures.

Table S1: surface composition of Mo-Ni catalysts by XPS measurements

$MoNiO_4$/Ni	Mo	Ni	O
Theoretical %	12.5	12.5%	75.0%
Theoretical Stoichiometry	1	1	6
Experimental %	10.6%	9.8%	79.6%
Experimental Stoichiometry	1.1	1.0	8.1

MoO_2/Ni (400)	Mo	Ni	O
Theoretical %	9.1%	18.2%	72.7%
Theoretical Stoichiometry	1	2	8
Experimental %	10.3%	16.2%	73.5%
Experimental Stoichiometry	1	1.6	7.1

MoO_2/Ni (500)	Mo	Ni	O
Theoretical %	8.3%	25.0%	66.7%
Theoretical Stoichiometry	1	3	8
Experimental %	8.2%	23.9%	67.9%
Experimental Stoichiometry	1.0	2.9	8.3

MoO_2/Ni (600)	Mo	Ni	O
Theoretical %	5.3	26.3%	68.4%
Theoretical Stoichiometry	1	5	12
Experimental %	5.3%	25.1%	69.6%
Experimental Stoichiometry	1	4.7	13

MoO_2/Ni (700)	Mo	Ni	O
Theoretical %	3.2%	32.3%	64.5%
Theoretical Stoichiometry	1	10	20
Experimental %	3.2%	32.6%	64.3%
Experimental Stoichiometry	1	10.3	20.4

MoO_2/Ni (800)	Mo	Ni	O
Theoretical %	12.5%	12.5%	75.0%
Theoretical Stoichiometry	1	1	6
Experimental %	12.4%	13.2%	74.4%
Experimental Stoichiometry	1.0	1.1	6.0

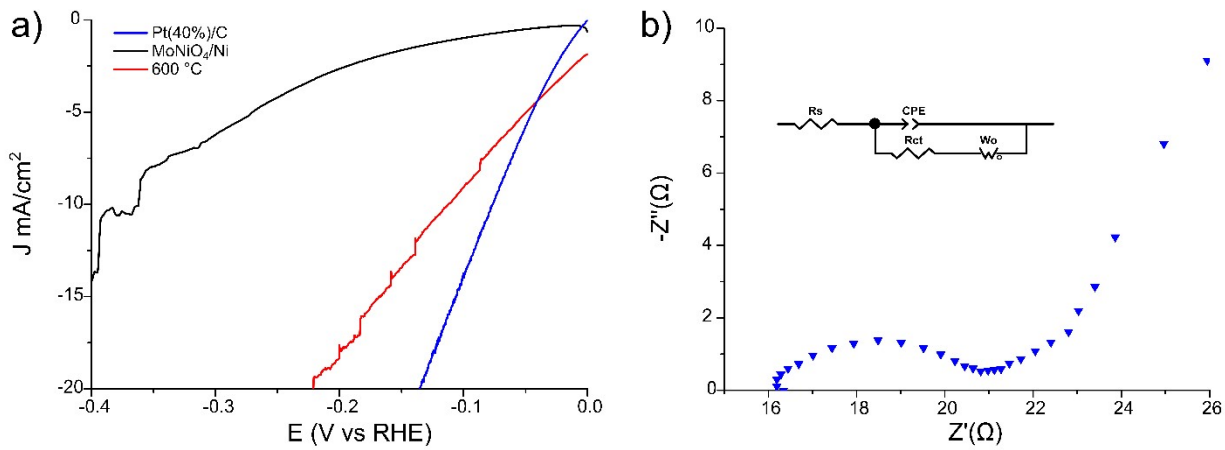


Figure S2: (a) LSV curves for HER of commercial Pt/C (40 wt%) Alfa Aesar, $MoNiO_4$/Ni, and MoO_2/Ni cathode treated at 600 °C; LSV scan from 0 to - 0.4 V (vs RHE) in H_2 sat KOH 0.1M at 1mV s^{-1}. (b) EIS of MoO_2/Ni 600 °C with equivalent circuit.

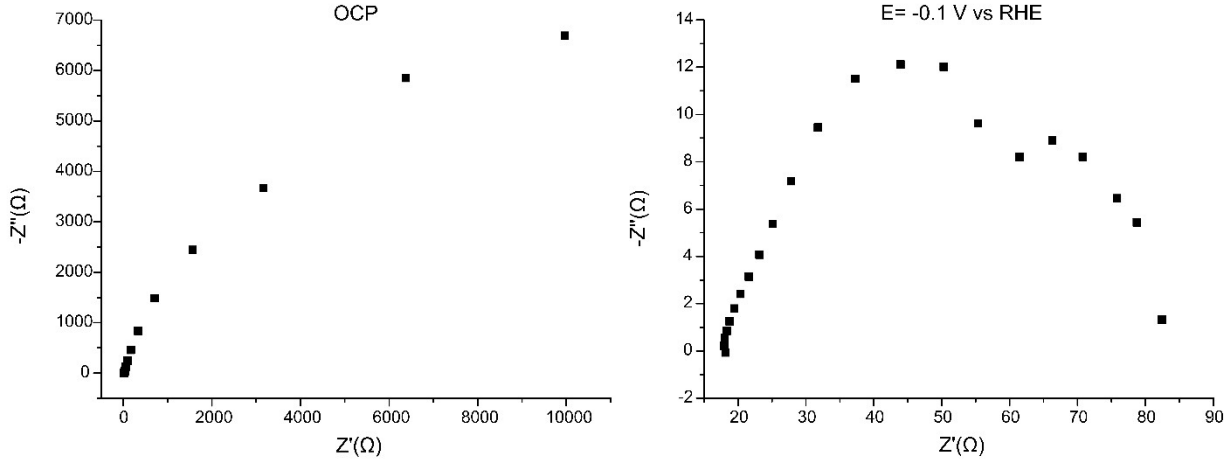


Figure S3: EIS of $MoNiO_4$/Ni at Open Circuit Potential (OCP) and -0.1 V vs RHE. KOH 0.1 M, in N_2 saturated solution.

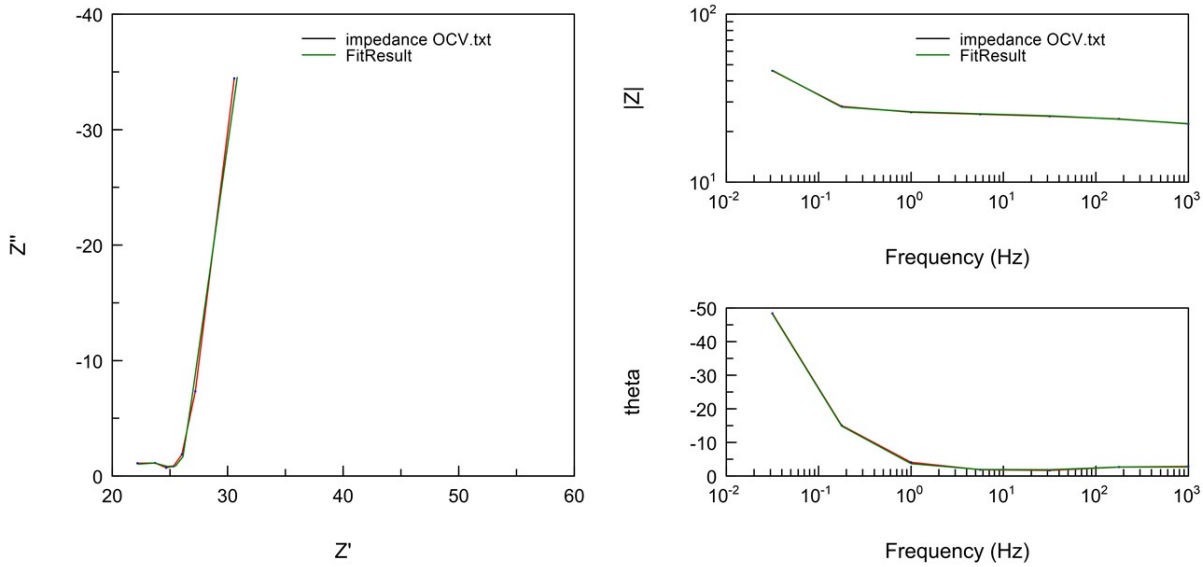


Figure S4: Nyquist plot and bode diagram for MoO_2/Ni (600) (red line), and fitting curve for the equivalent circuit (green line), at OCV condition.

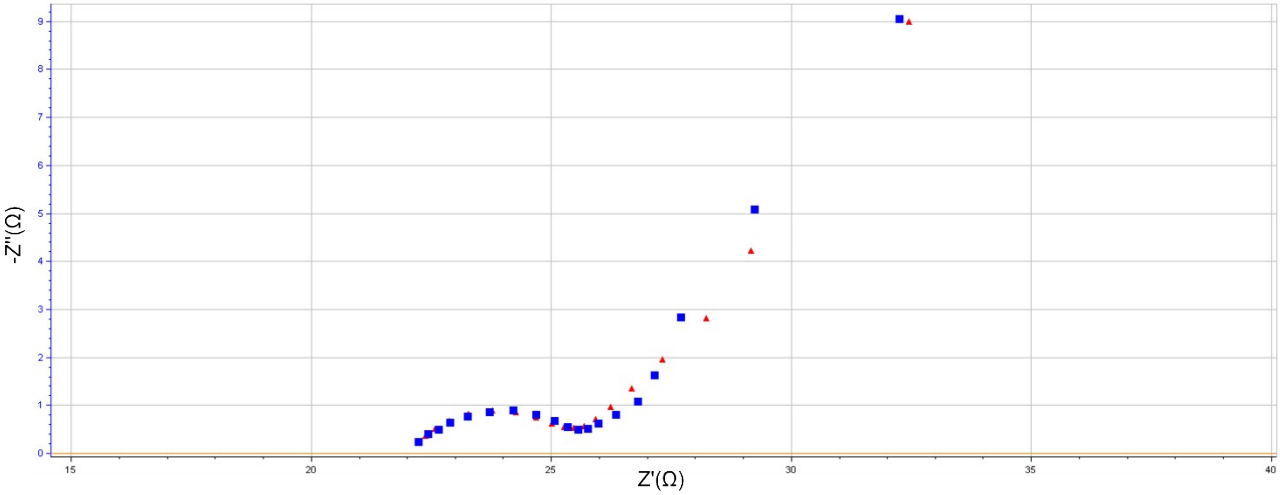


Figure S5: Nyquist plot for MoO_2/Ni (600) (blue squares), and fitting curve for the equivalent circuit (red triangles), at -0.1 V vs RHE.

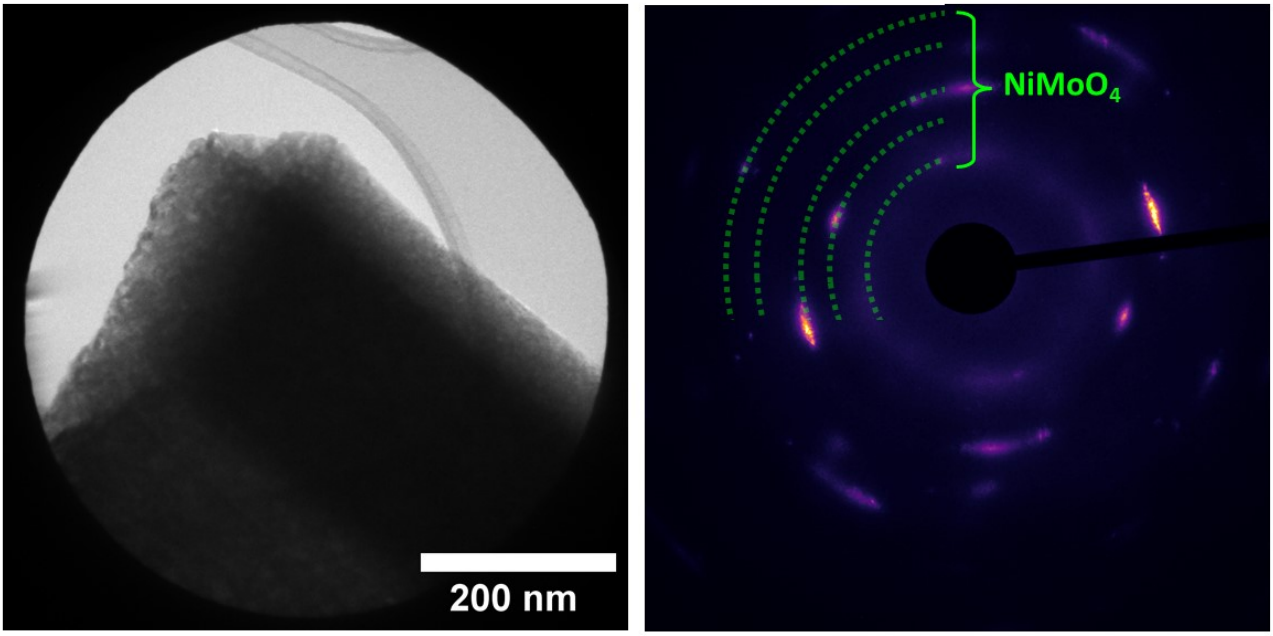


Figure S6: Selected Area (TEM micrograph) and related electron diffraction (false color) of sample prepared at 400 °C MoO_2/Ni. Main diffraction rings were indexed as $NiMoO_4$ (-1 1 1); (-1 2 0); (-1 2 2); (-1 2 3) and (0 -2 3) (from the center to the border).

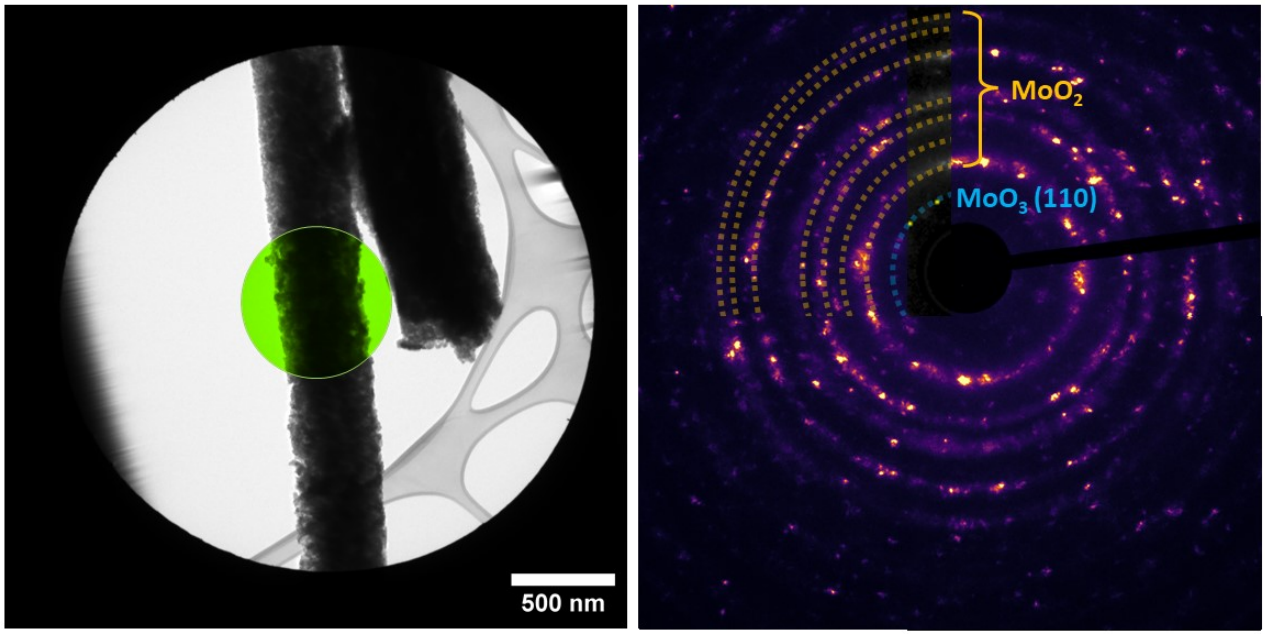


Figure S7: Representative TEM micrograph, selected Area (highlighted in green) and related electron diffraction (false color) of sample MoO_2-Ni (600). Main diffraction rings were indexed as MoO_2 (1 1 0); (1 -1 2); (2 0 0); (1 2 0) ; (2 2 0) ; (1 -2 4) and (2 3- 1) (from the center to the border).

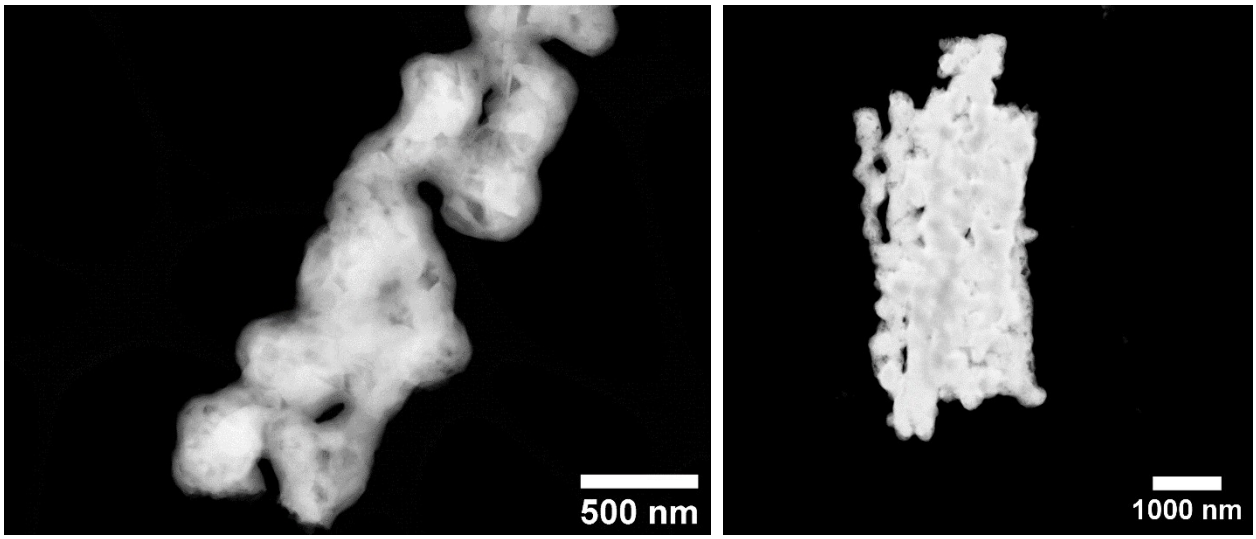


Figure S8: Representative STEM micrographs of sample MoO_2/Ni (800).

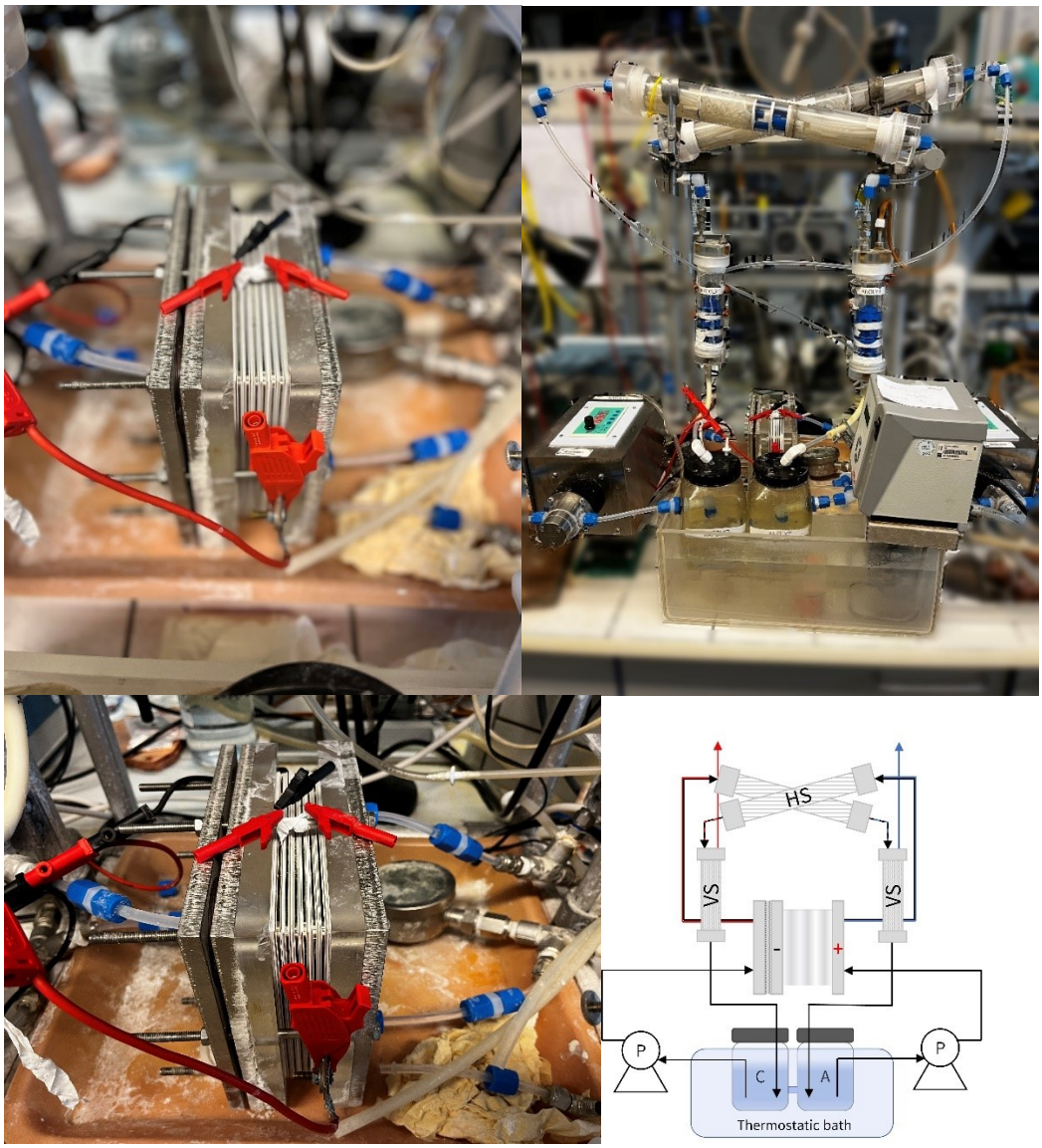
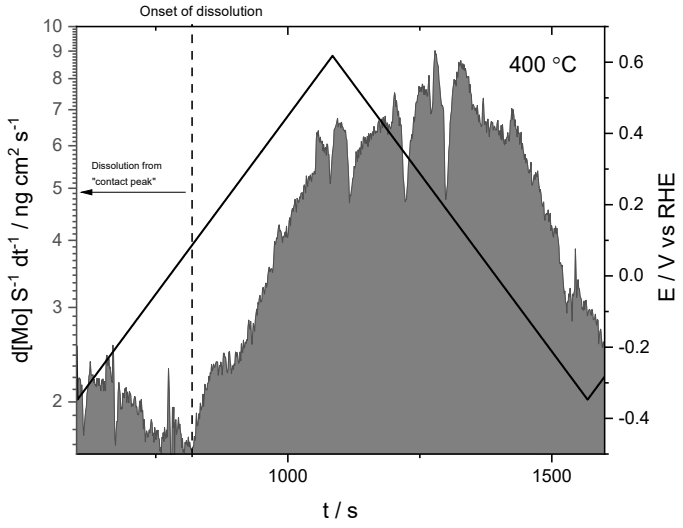


Figure S9: Zero-Gap Laboratory-Scale Anion Exchange Membrane Alkaline Water Electrolysis 3 cell Stack. Electrode active surface area 78.5 cm^2.

Table S2: Total dissolution and dissolution without contact peak, with relative E_{onset} recorded in the first CV for the MoO_2/Ni series. Figure shows an example of how the onset potential was estimated.



	Total dissolution (ng cm^{-2})	Dissolution (without contribution from contact peak) (ng cm^{-2})	E_{onset} 1st CV (V vs RHE)
Catalyst	Mo		
400 °C	13386	7168	0.088
500 °C	10781	3618	-0.031
600 °C	6076	704	0.242
700 °C	10582	2911	0.185

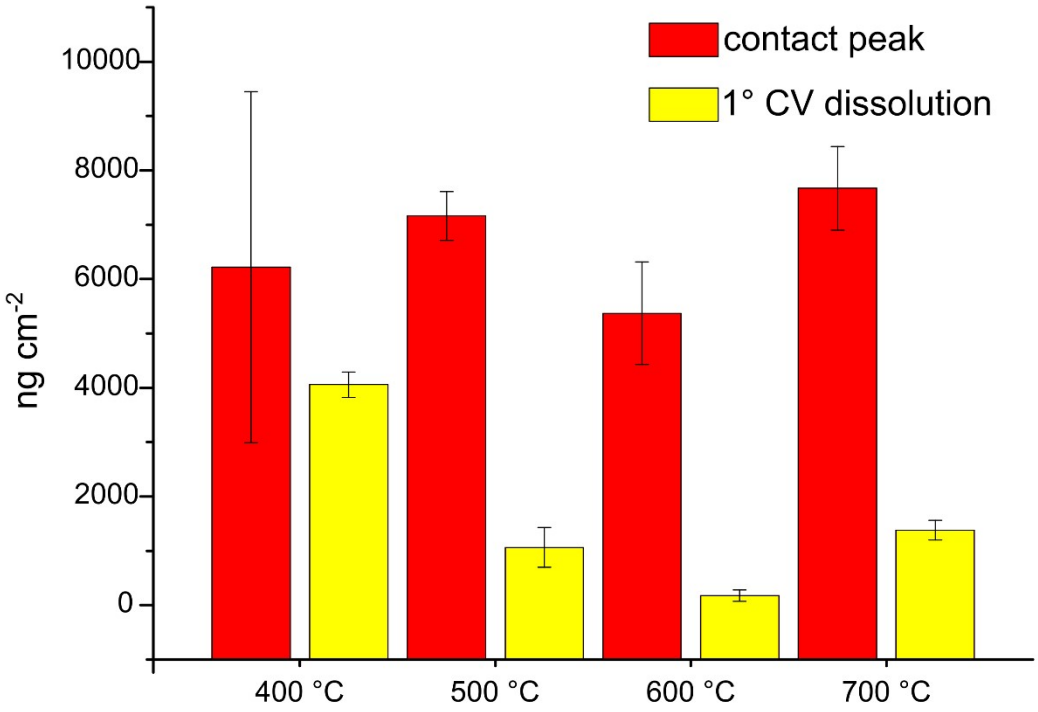


Figure S10: Dissolved amounts calculated by integrating the dissolution profiles of MoO_2/Ni cathodes, with error bars.

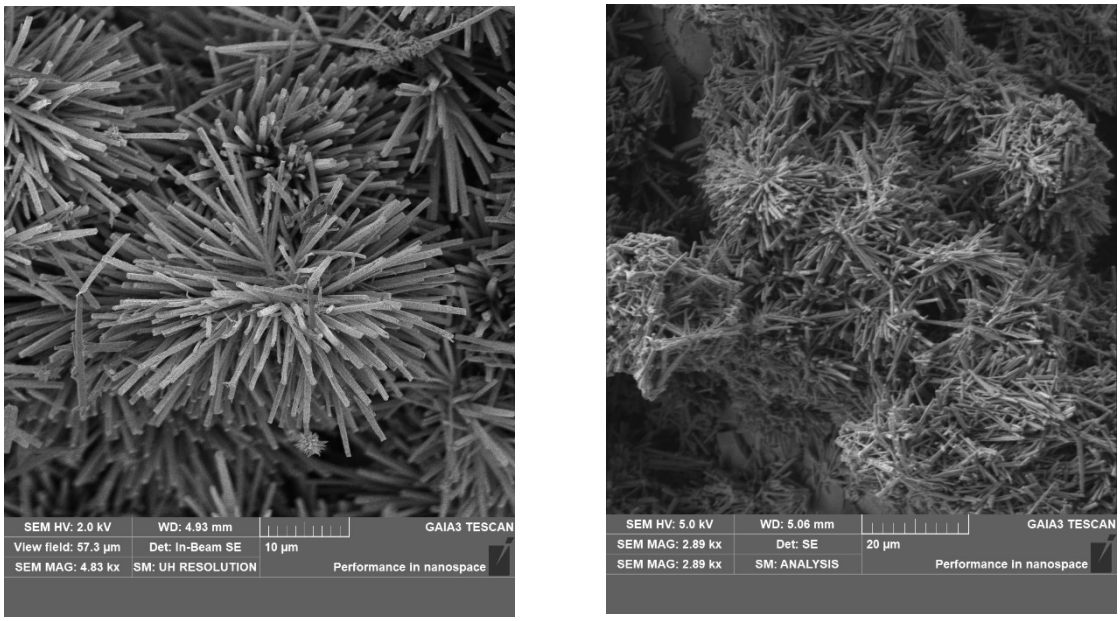


Figure S11: SEM images of MoO_2/Ni (600 °C) cathode, before (left) and after 2-week cell test (right).

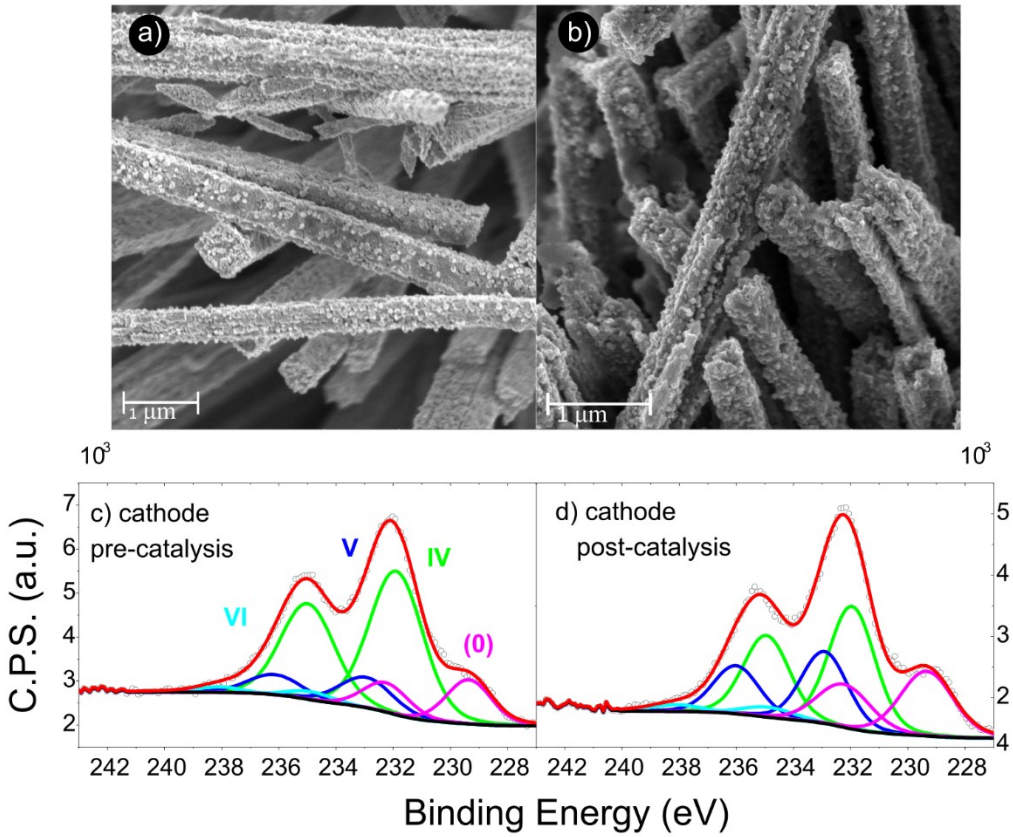


Figure S12: SEM images of MoO_2/Ni (600) (a) pre-catalysis (b) post-2 week cell test. Mo XPS spectra (c) pre-catalysis, (d) post-2 weeks cell test.

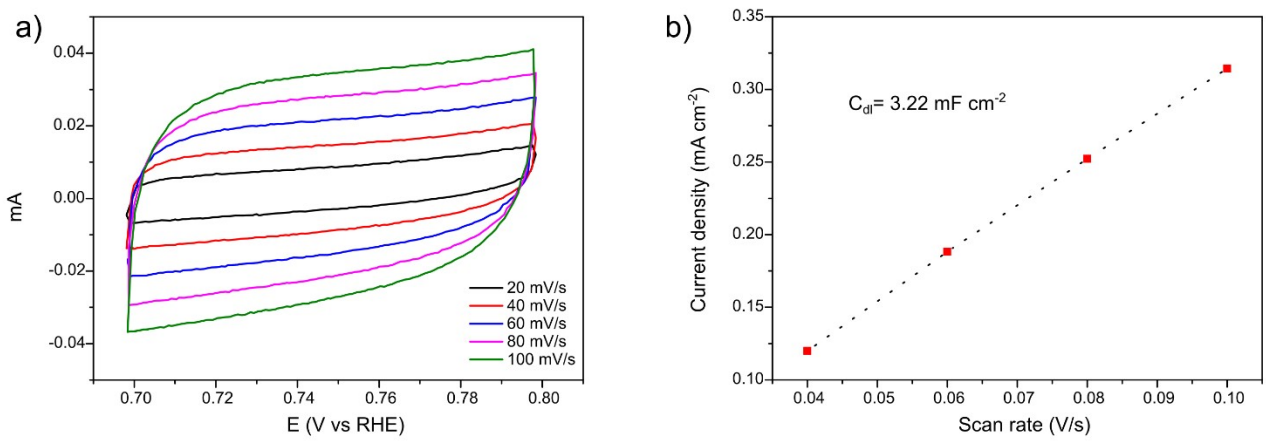


Figure S13: Electrochemical capacitance measurement for MoO_2/Ni. a) CVs were recorded in a potential range (0.7-0.8 V vs.RHE) without faradaic processes. b) Cdl (Capacitance double layer) were obtained by the slope of the capacitive current determined at 0.75 V as a function of scan rate.

Table S3: C_{dl} (Double Layer Capacitance) comparison with other reported in literature.

Catalysts	Cdl	Reference
MoO_2/Ni (600 °C)	3.22 mF cm^{-2}	This work
$Ni_{foam}/Ni_4Mo:MoO_2$	2.25 mF cm^{-2}	[1]
$MoNi_4@MoO_{3-x}$	0.45 mF cm^{-2}	[2]

Table S4: Performance comparison of literature AEMWE data with Ni-Mo cathodes.

Anion Exchange Membrane	**Anion Exchange Ionomer**	**Cathode Catalyst**	**Anode catalyst**	**Electrolyte**	**Cell temp. °C**	**A cm^{-2}@ V_{cell}**	**Durability data**	**Ref.**
FAA-3-PK130	--	MoO_2/Ni	Fe-Mo-Ni/Ni	1M KOH @anode	60	0.55@2	300h 0.5 A cm^{-2}	This work
PTFE-Sustainion	Nafion	Ni-Mo	Fe-Ni-Mo	1M KOH @cathode	80	1.0@1.57	--	[3]
FAA-3–50	FAA3	NiMo/KB	NiFe (85:15 at.%)	1M KOH @anode	50	1.0@1.8	2000h 1 A cm^{-2}	[4]
PVBC-MPy/35%PEK-cardo	--	Ni-Mo	Ni-Fe	1M KOH	60	0.5@2	42h 0.5 A cm^{-2}	[5]

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