Supporting Information

Hybrid nanostructured compounds of Mo_2C on vertical graphene nanoflakes for a highly efficient hydrogen evolution reaction.

Stefanos Chaitoglou[1,2*], Roger Amade[1,2], Rogelio Ospina[3], Enric Bertran-Serra[1,2]

*Corresponding Author: Dr. Stefanos Chaitoglou

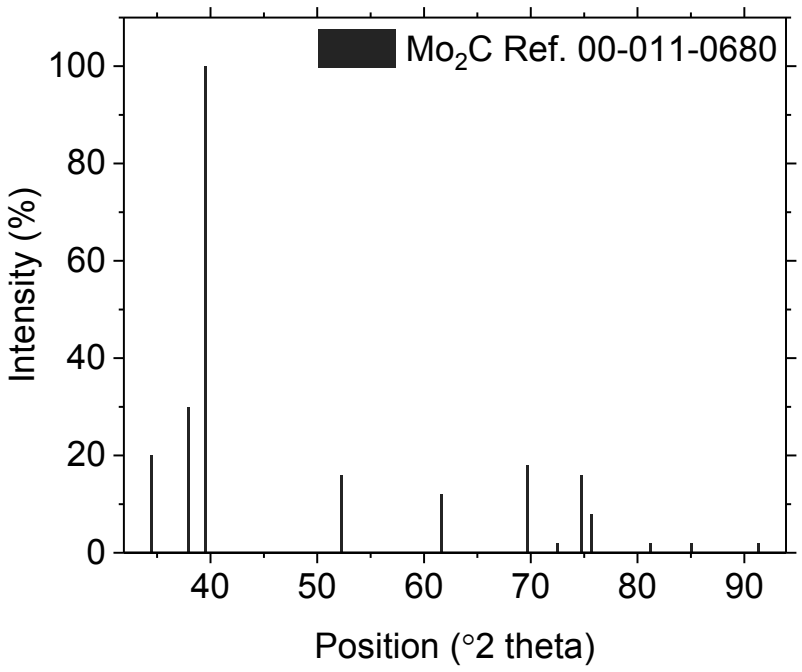
Contact email: stefanoschaitoglou@ub.edu

1. Department of Applied Physics, University of Barcelona, C/Martí i Franquès, 1, 08028 Barcelona, Catalunya, Spain

2. ENPHOCAMAT Group, Institute of Nanoscience and Nanotechnology (IN2UB), Universitat de Barcelona, C/Martí i Franquès, 1, 08028 Barcelona, Catalunya, Spain

3. Escuela de Física, Universidad Industrial de Santander, Carrera 27 calle 9 Ciudad Universitaria Bucaramanga, Colombia

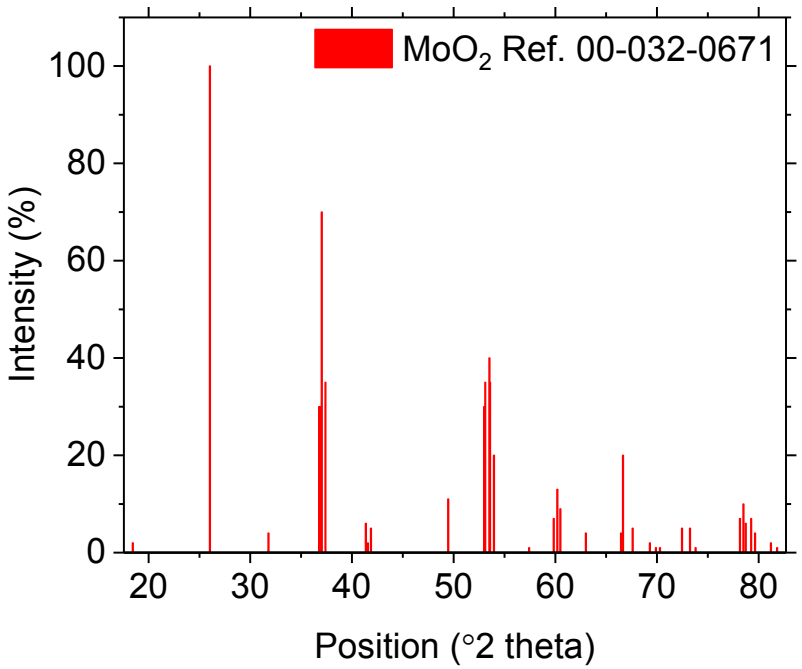
Supplementary figures



Peak list Mo_2C

No.	h	k	l	d [A]	2Theta[deg]	I [%]
1	1	0	0	2.60000	34.467	20.0
2	0	0	2	2.37000	37.934	30.0
3	1	0	1	2.28000	39.492	100.0
4	1	0	2	1.75000	52.230	16.0

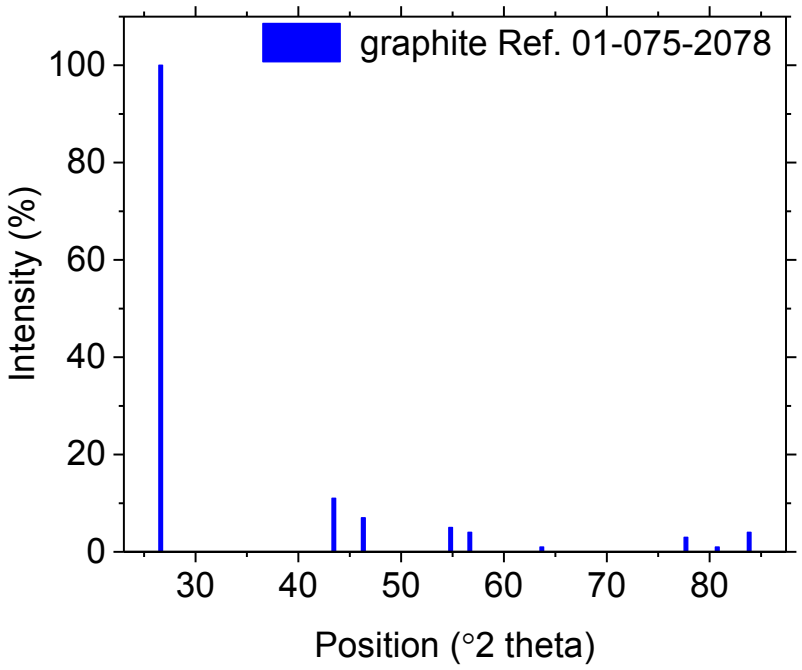
5	1	1	0	1.50300	61.662	12.0
6	1	0	3	1.34900	69.642	18.0
7	2	0	0	1.30300	72.481	2.0
8	1	1	2	1.26900	74.748	16.0
9	2	0	1	1.25500	75.727	8.0
10	0	0	4	1.18300	81.255	2.0
11	2	0	2	1.14000	85.017	2.0
12	1	0	4	1.07700	91.324	2.0
13	2	0	3	1.00300	100.349	2.0
14	2	1	0	0.98400	103.040	2.0
15	2	1	1	0.96400	106.082	4.0
16	1	1	4	0.93000	111.845	4.0
17	2	1	2	0.90800	116.065	2.0
18	1	0	5	0.89000	119.881	2.0
19	2	0	4	0.87500	123.367	2.0
20	3	0	0	0.86800	125.107	2.0
21	2	1	3	0.83500	134.593	4.0
22	3	0	2	0.81500	141.872	2.0



Peak list MoO_2

No.	h	k	l	d [A]	2Theta[deg]	I [%]
1	-1	0	1	4.80500	18.450	2.0
2	-1	1	1	3.42000	26.033	100.0
3	1	0	1	2.81300	31.785	4.0
4	2	0	0	2.44200	36.775	30.0
5	1	1	1	2.43700	36.853	30.0
6	-2	1	1	2.42600	37.026	70.0
7	-2	0	2	2.40300	37.393	35.0
8	2	1	0	2.18100	41.365	6.0

9	0	2	1	2.17100	41.564	2.0
10	-2	1	2	2.15600	41.867	5.0
11	-3	0	1	1.84100	49.469	11.0
12	2	1	1	1.72500	53.045	30.0
13	-2	2	0	1.72300	53.112	35.0
14	-3	1	2	1.71100	53.514	40.0
15	-2	2	2	1.70900	53.581	35.0
16	-2	1	3	1.69760	53.970	20.0
17	-3	0	3	1.60330	57.429	1.0
18	-3	1	0	1.54430	59.842	7.0
19	0	3	1	1.53600	60.198	13.0
20	0	1	3	1.52720	60.581	9.0
21	-3	2	1	1.46760	63.319	4.0
22	2	0	2	1.40570	66.458	4.0
23	-4	0	2	1.40190	66.661	20.0
24	-2	0	4	1.38450	67.611	5.0
25	3	0	1	1.35480	69.301	2.0
26	0	3	2	1.34480	69.891	1.0
27	-3	2	3	1.33810	70.293	1.0
28	-4	1	1	1.30330	72.461	5.0
29	-4	1	3	1.29120	73.250	5.0
30	-3	1	4	1.28290	73.802	1.0
31	4	0	0	1.22190	78.161	7.0
32	2	3	1	1.21750	78.498	10.0
33	1	3	2	1.21460	78.721	6.0
34	-2	3	3	1.20760	79.267	7.0
35	-2	2	4	1.20280	79.647	4.0
36	3	2	1	1.18370	81.197	2.0
37	1	2	3	1.17640	81.808	1.0
38	-3	3	0	1.14850	84.242	2.0
39	0	3	3	1.14140	84.889	4.0



Peak list graphite

No.	h	k	l	d [A]	2Theta[deg]	I [%]
1	1	1	1	3.34701	26.611	100.0
2	0	1	0	2.08083	43.455	11.3
3	1	1	0	1.95849	46.322	7.2
4	2	2	2	1.67351	54.812	5.0
5	1	1	2	1.62279	56.677	4.0
6	2	2	1	1.46021	63.677	1.4
7	-1	1	0	1.22803	77.697	3.2
8	2	3	2	1.18926	80.739	1.0
9	1	2	0	1.15288	83.849	4.9
10	3	3	3	1.11567	87.329	0.7

Figure S1: Data of the JCPDS patterns of graphite (bottom), MoO_2 (middle) and a-Mo_2C (top).

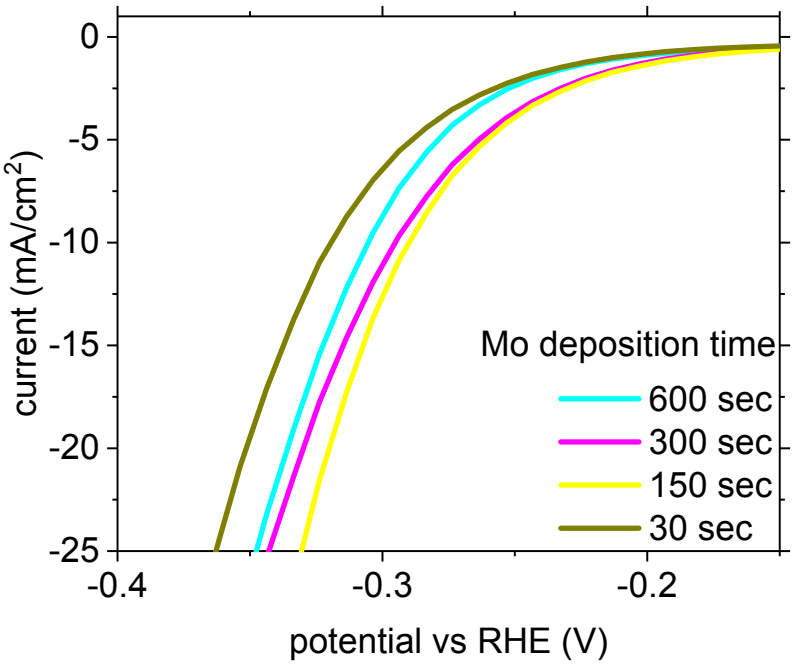


Figure S2: Linear sweel voltammetry curves of Mo deposited on GNWs/ Papyex ®, under various deposition times

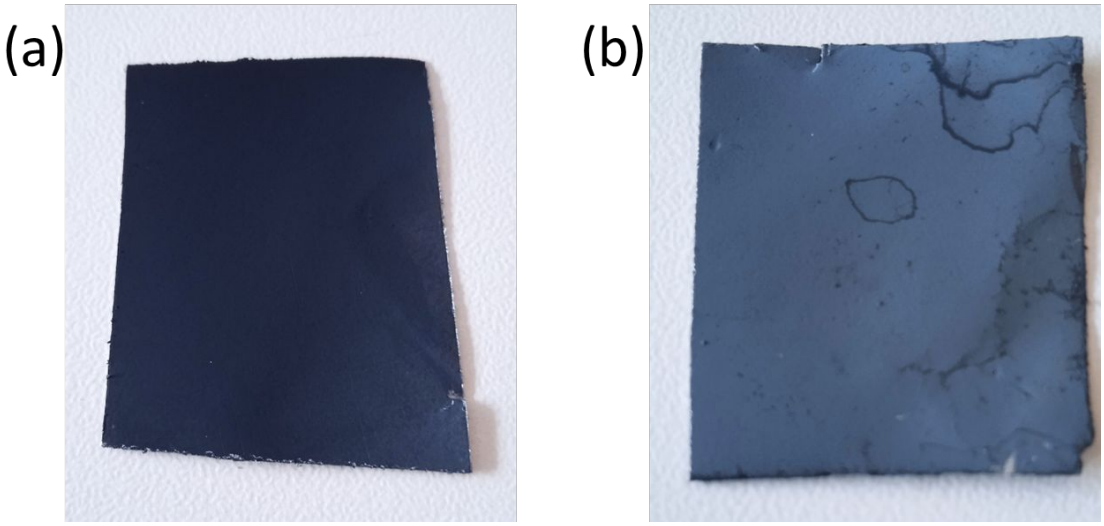
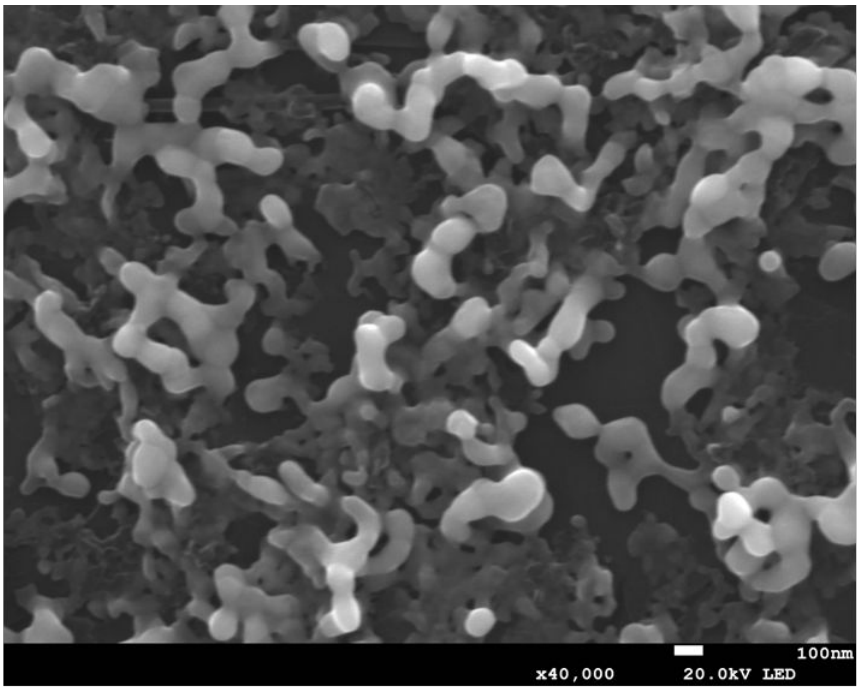


Figure S3: Digital image of a) GNWs on Papyex electrode and b) nanostructured Mo_2C on GNWs electrode.


100nm
x40,000
20.0kV LED

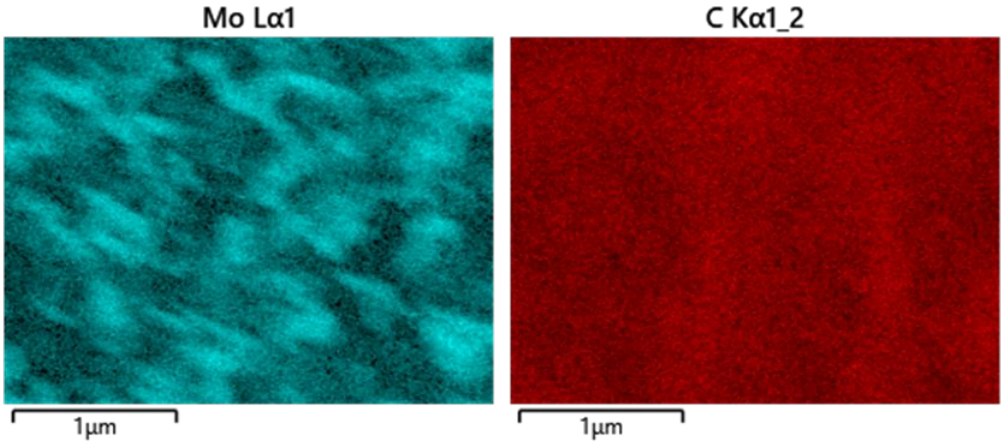

Mo Lα1
C Kα1_2
1μm
1μm

Figure S4: Mo and C EDS mapping and SEM image of Mo_2C/GNWs prepared after 15 min of annealing times.

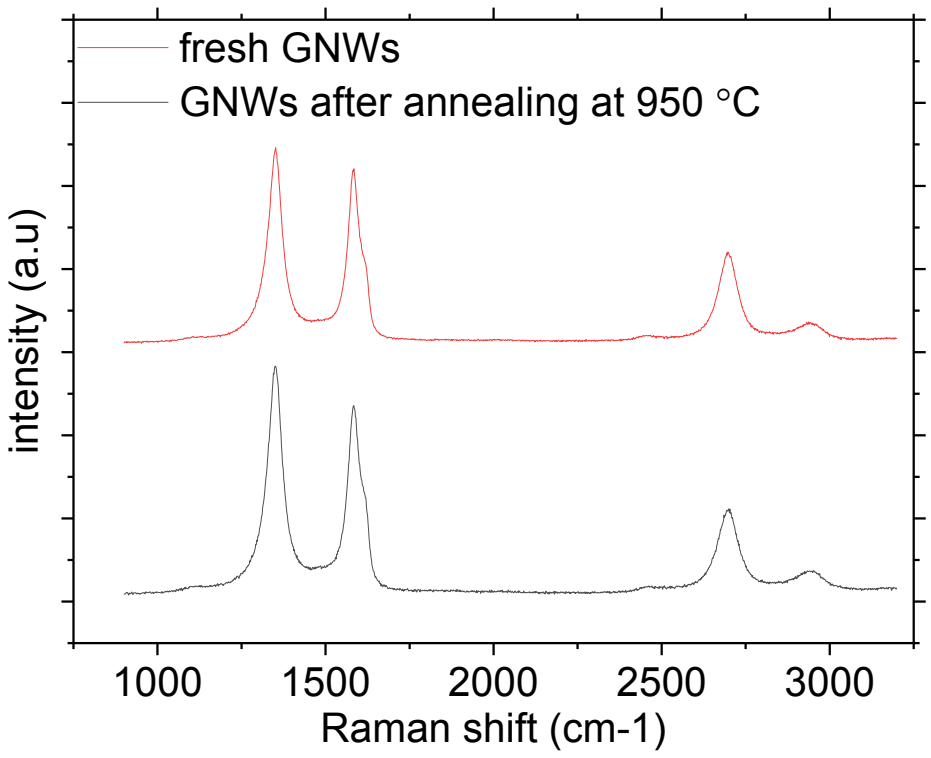


Figure S5: Raman spectra of bare GNWs, fresh (red line) and after thermal annealing at 950 ˚C (black line) in Ar atmosphere, showing luck of any structural alteration.

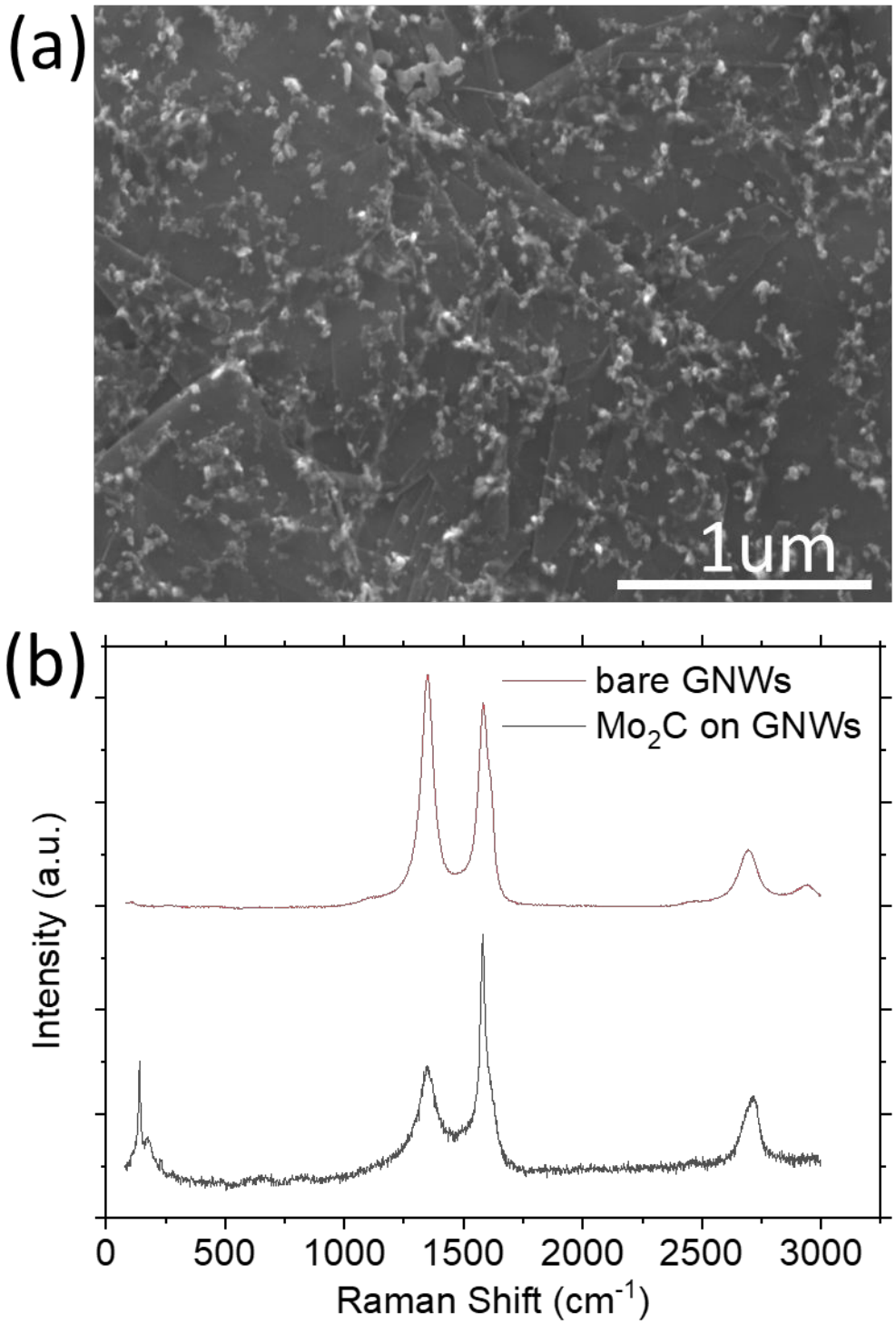


Figure S6: a) SEM image of Mo_2C deposited on GNWs/Papyex ©, after carburization in CH_4 atmosphere. Partial etching of the GNWs is observed. b) Raman spectra of the sample before

and after Mo_2C deposition reveal the deterioration in the crystal quality of the GNWs, as a result of the carburization process in CH_4 atmosphere.

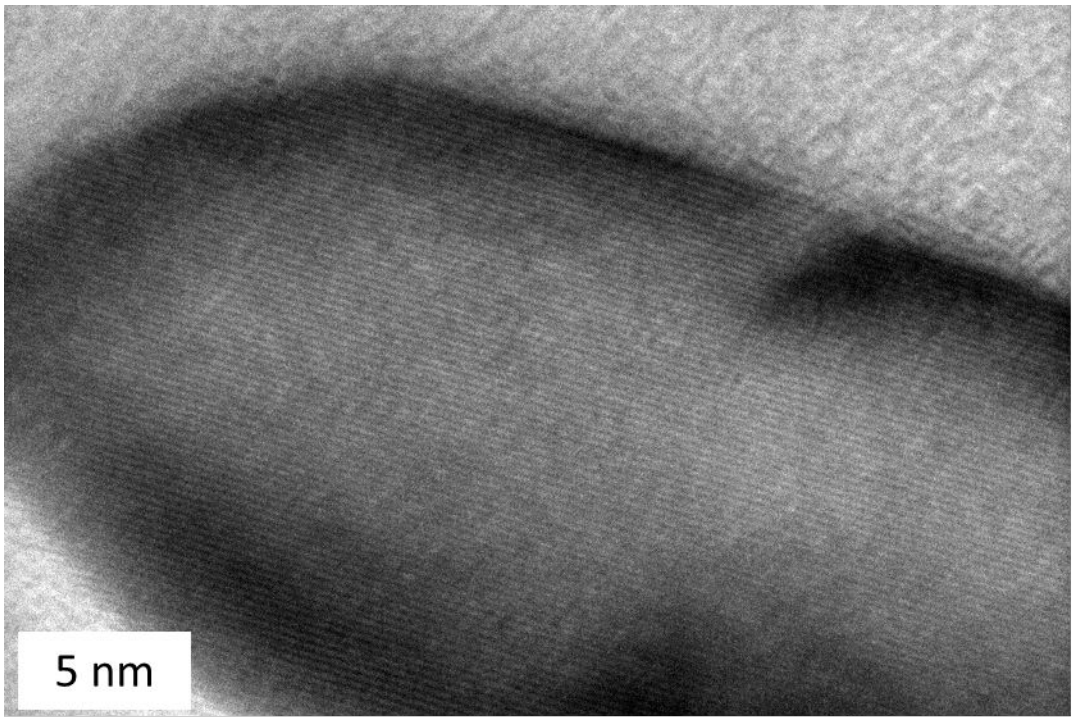


Figure S7: TEM image of a single crystal Mo_2C particle.

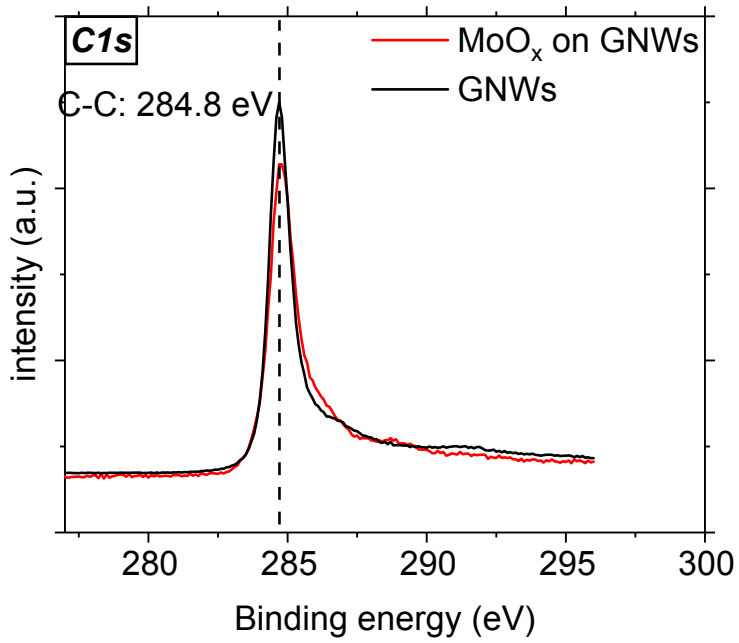


Figure S8: XPS graph of C_{1s} peak of GNWs/ Papyex and Mo deposited on GNWs on Papyex , revealing absence of Mo-C interaction.

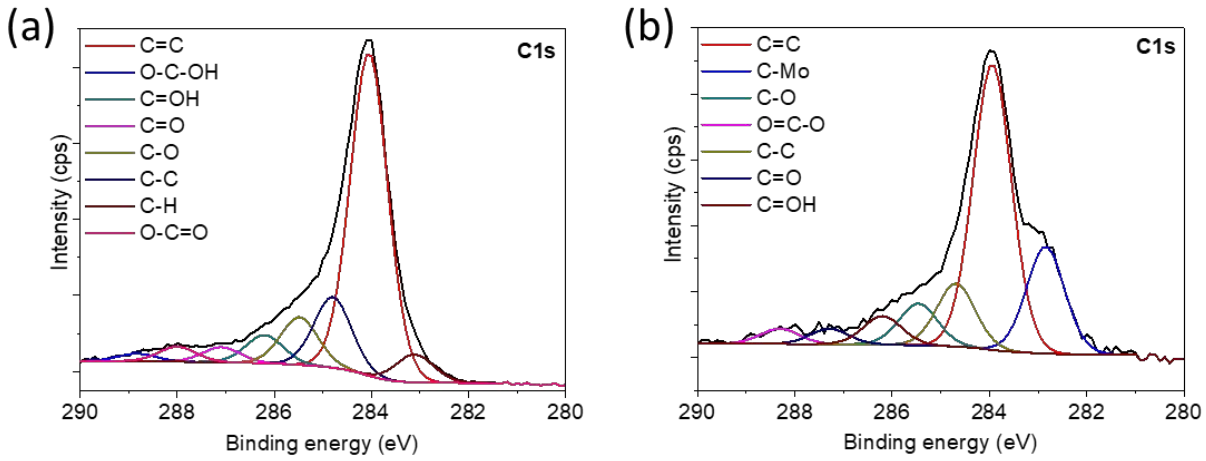


Figure S9: XPS graph of C_{1s} peak a) before and b) after carburization.

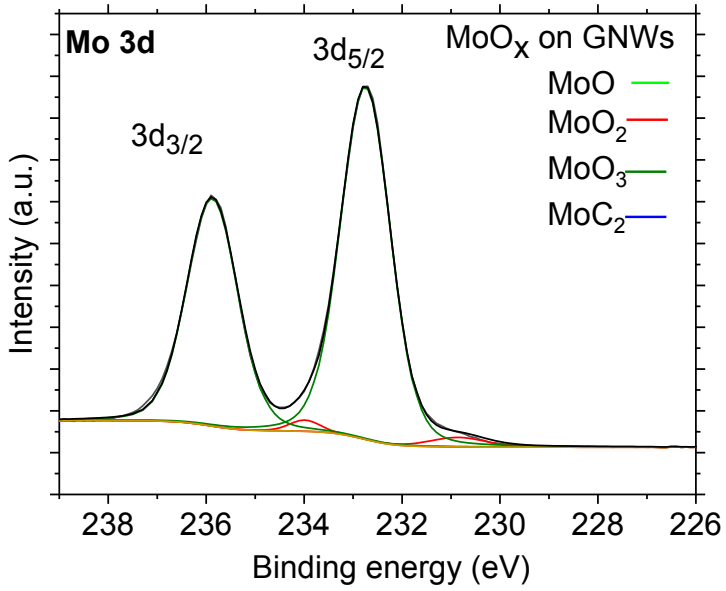


Figure S10: XPS graph of Mo3d peak before carburization.

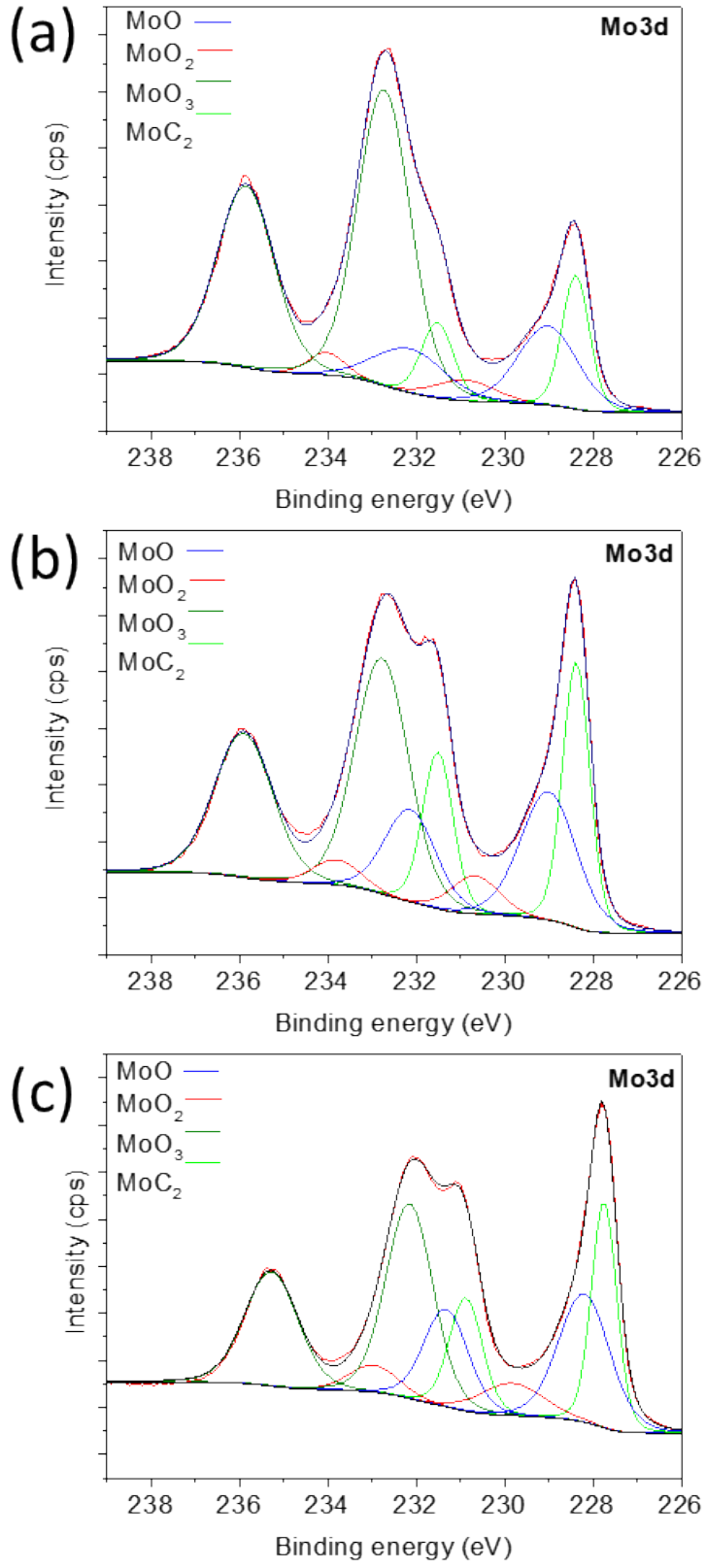


Figure S11: XPS graph of Mo_{3d} peak after 4' (a), 8' (b) and 15' (c) of carburization duration.

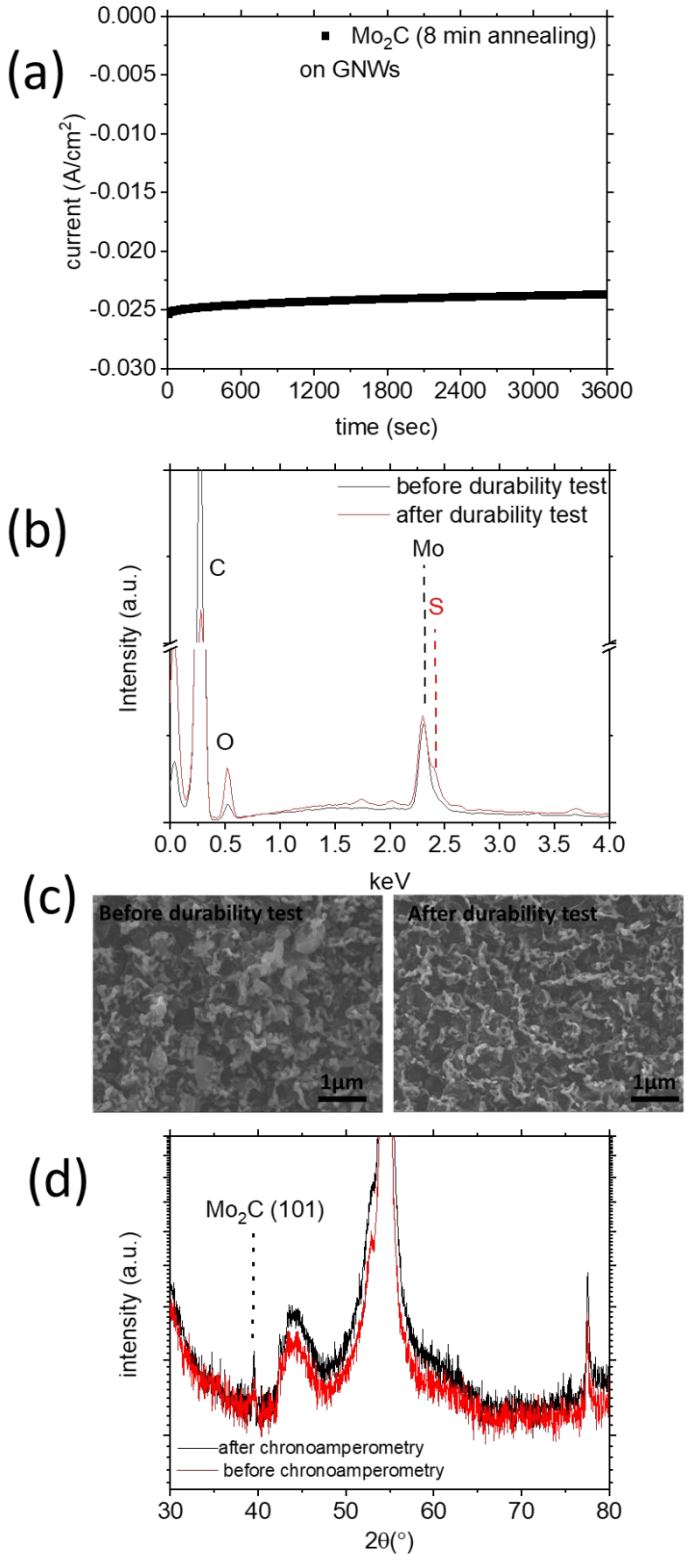


Figure S12: a) Chronoamperometry test during 1 h under 200 mV of constant bias vs RHE. b) EDS analysis, c) SEM images and d) XRD analysis, of the electrode before and after the test

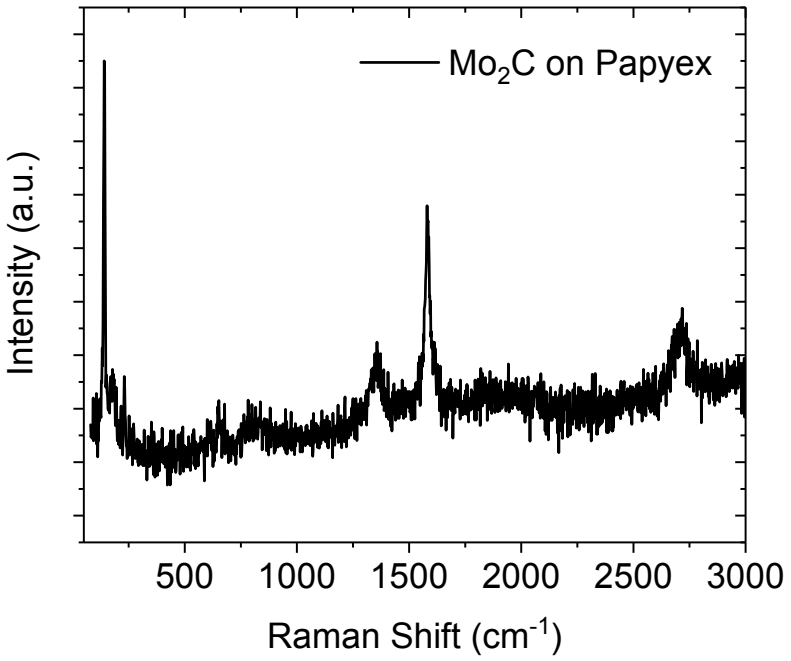


Figure S13: Raman spectrum of Mo_2C on Papyex substrate.

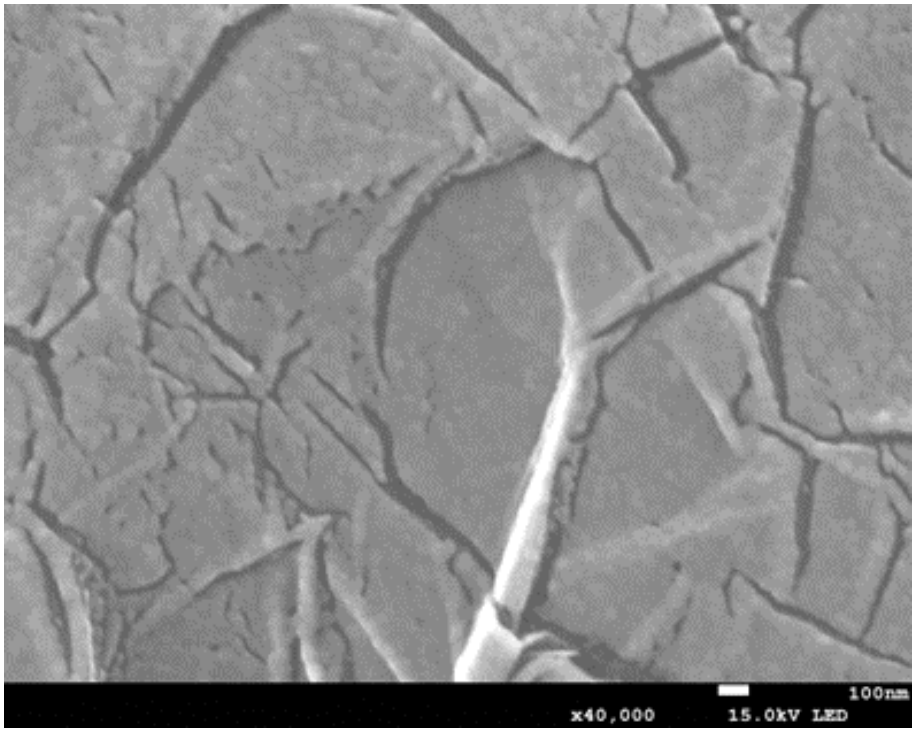


Figure S14: SEM image of a Mo_2C film formed on a Papyex substrate, after carburization of sputtered Mo in a CH_4 atmosphere.

.

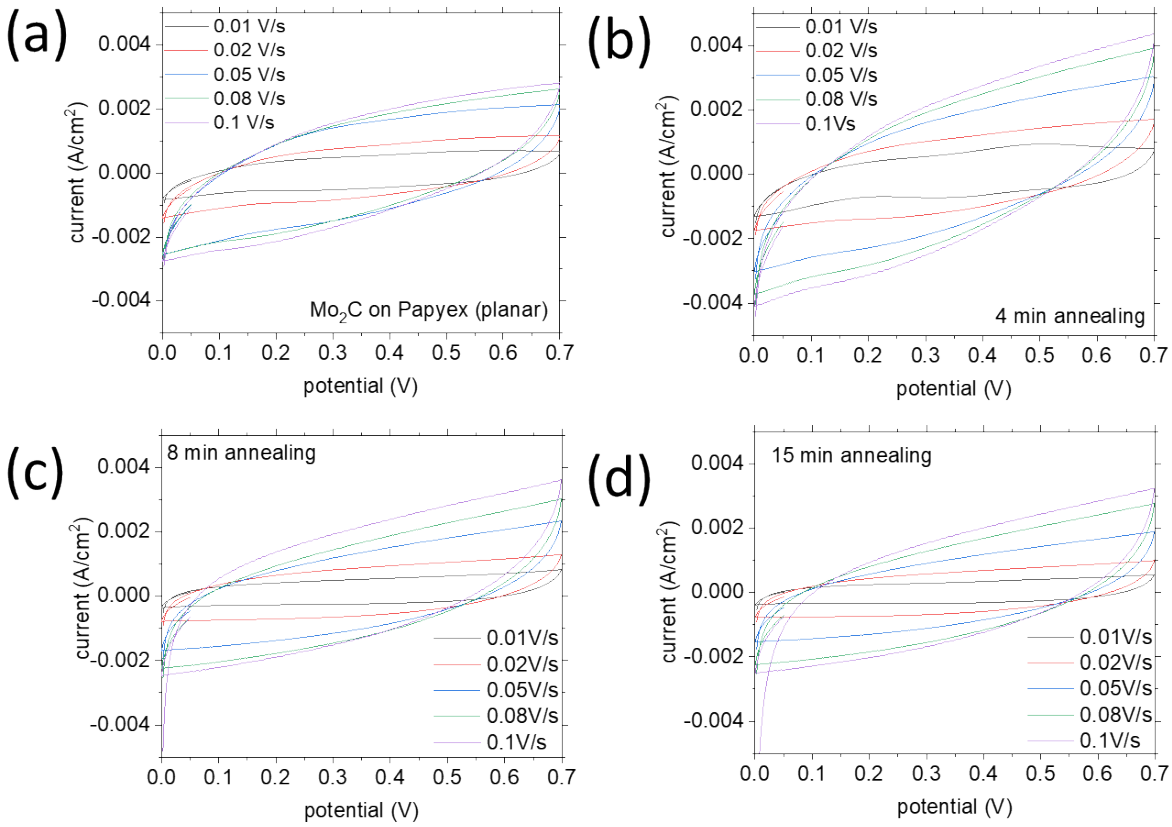


Figure S15: CV graphs of Mo carbide deposited on a) Papyex and GNWs after b) 4', c) 8' and c) 15' of annealing duration, obtained under varying scan rates

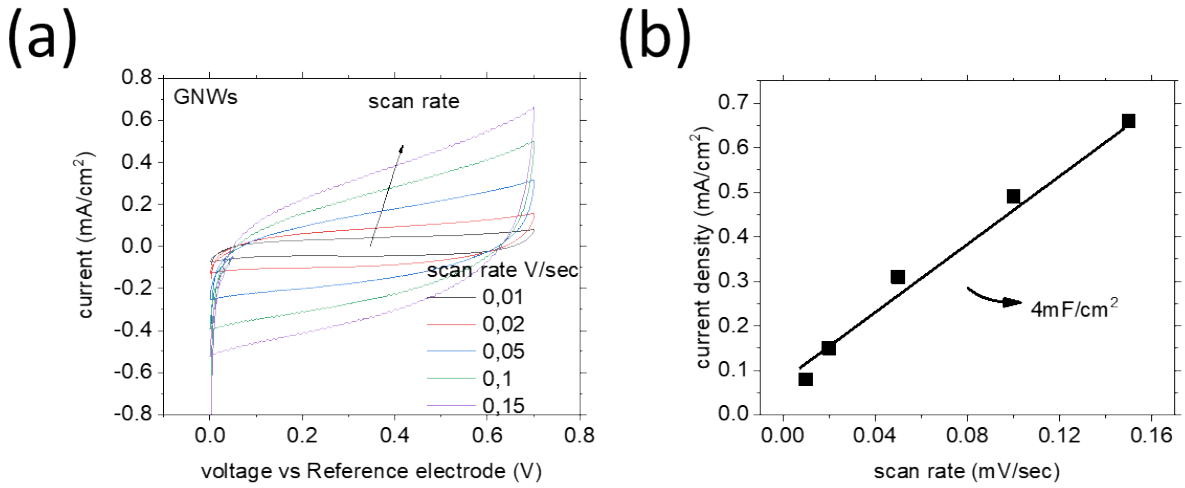


Figure S16: a) CV graphs and b) current density-scan rate plots of bare GNWs electrodes.