Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Rich-grain-boundary Ni_3Se_2 nanowire arrays as multifunctional electrode for electrochemical energy conversion and storage

Xin Shi,[a] Hui Wang,[a] Palanisamy Kannan,[b] Jieting Ding,[a] Shan Ji,*[ab] Fusheng Liu,*[a] Hengjun Gai,[a] and Rongfang Wang*[a]

[a] College of Chemical Engineering, Qingdao University of Science and Technology, Qingdao, 266042, China

[b] College of Biological, Chemical Science and Chemical Engineering, Jiaxing University, Jiaxing, 314001, China

***Corresponding authors:**

Shan Ji (*): jishan@mail zjxu.edu.cn, Tel./fax: +86 (0)15024355548

Fusheng Liu (*): liufusheng63@sina.com, Tel./fax: +86 (0)15192559078

Rongfang Wang (*): rfwang@qust.edu.cn, Tel./fax: +86(0)13919839172

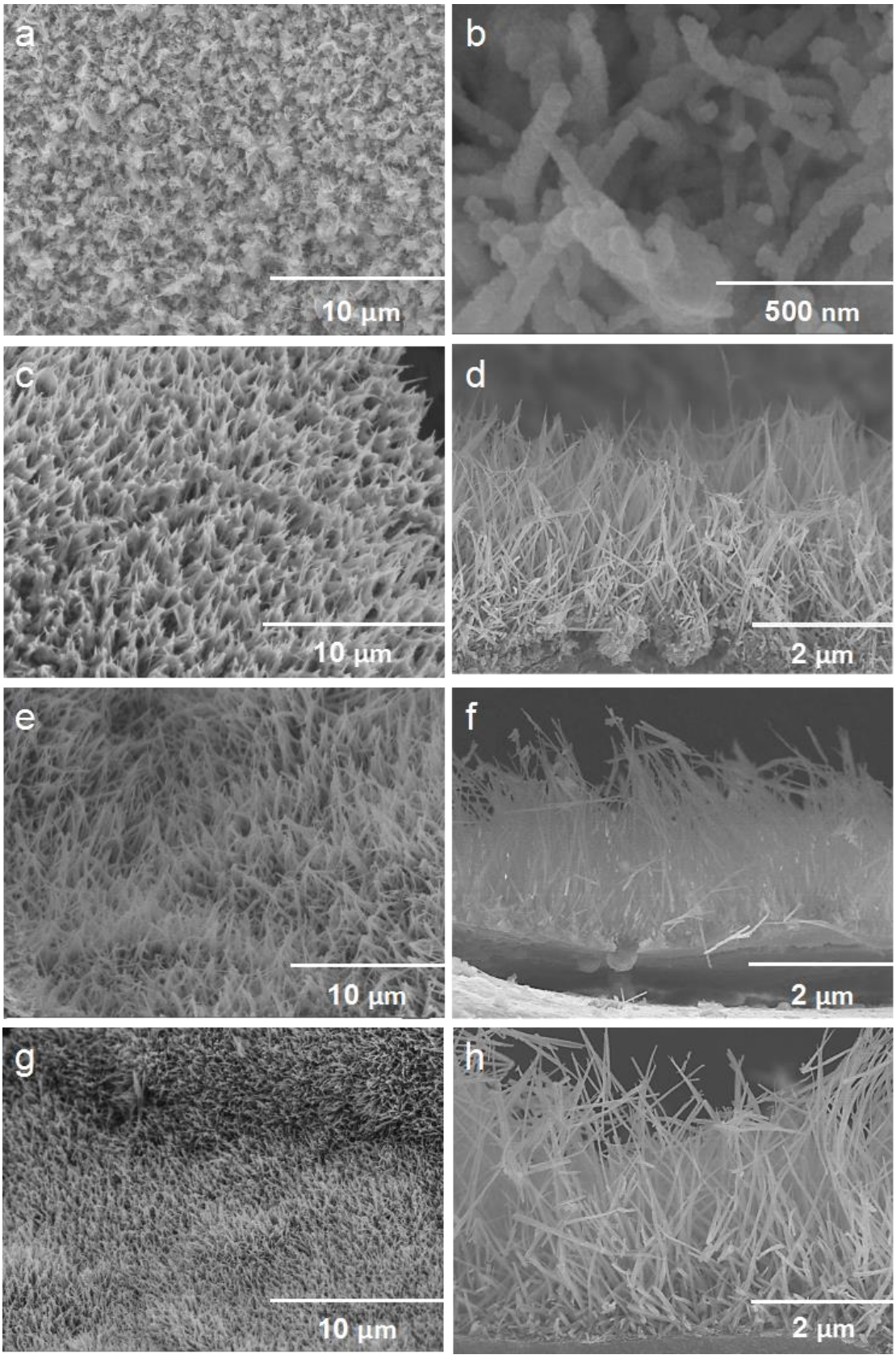

Figure S1. SEM images of Ni_3Se_2/NF-0.2 (a, b), Ni_3Se_2/NF-0.3 (c, d), Ni_3Se_2/NF-0.5 (e, f) and Ni_3Se_2/NF-0.6 (g, h).

Figure S2. Picture showing the destruction of Ni foam while using 0.7 mmol Se powder for Ni_3Se_2/NF nanowire arrays.

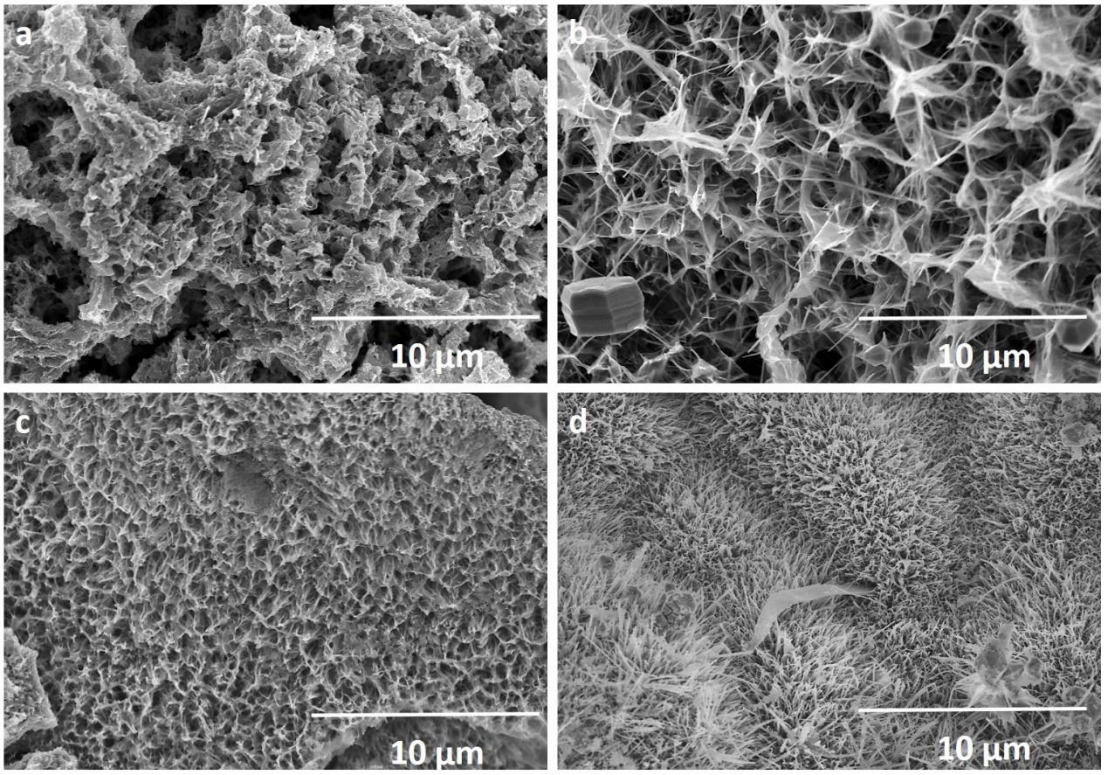

Figure S3. SEM images of nickel selenide prepared with different reaction time, (a) 6 h, (b) 12 h, (c) 18 h and (d) 24 h.

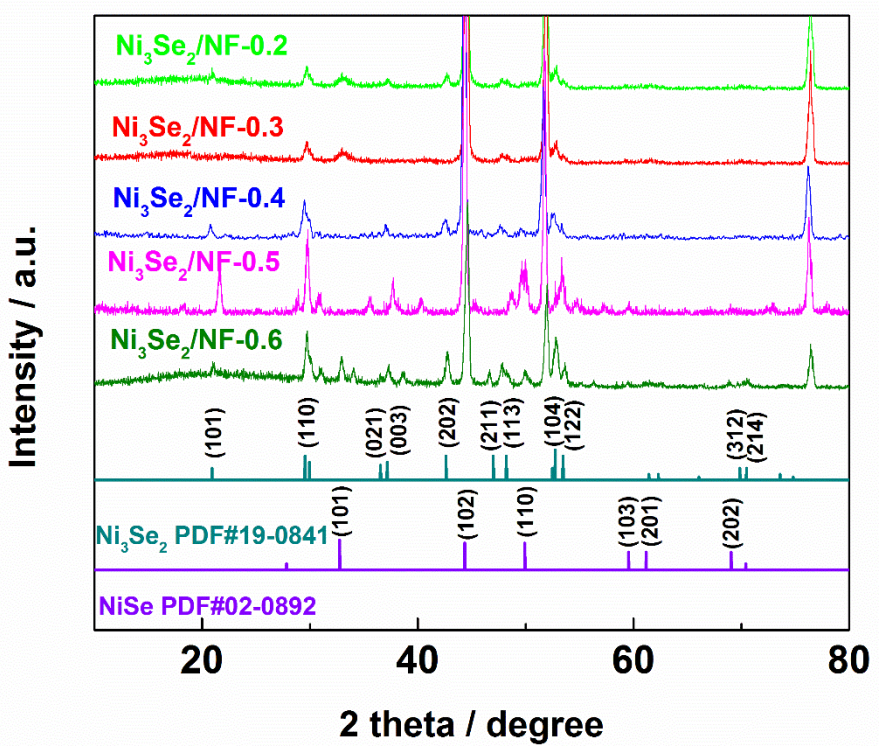

Figure S4. XRD patterns obtained for Ni_3Se_2/NF samples with Se powder concentration of 0.2 (fluorescent line), 0.3 (red line), 0.4 (blue line), 0.5 (pink line), and 0.6 mmol (green line).

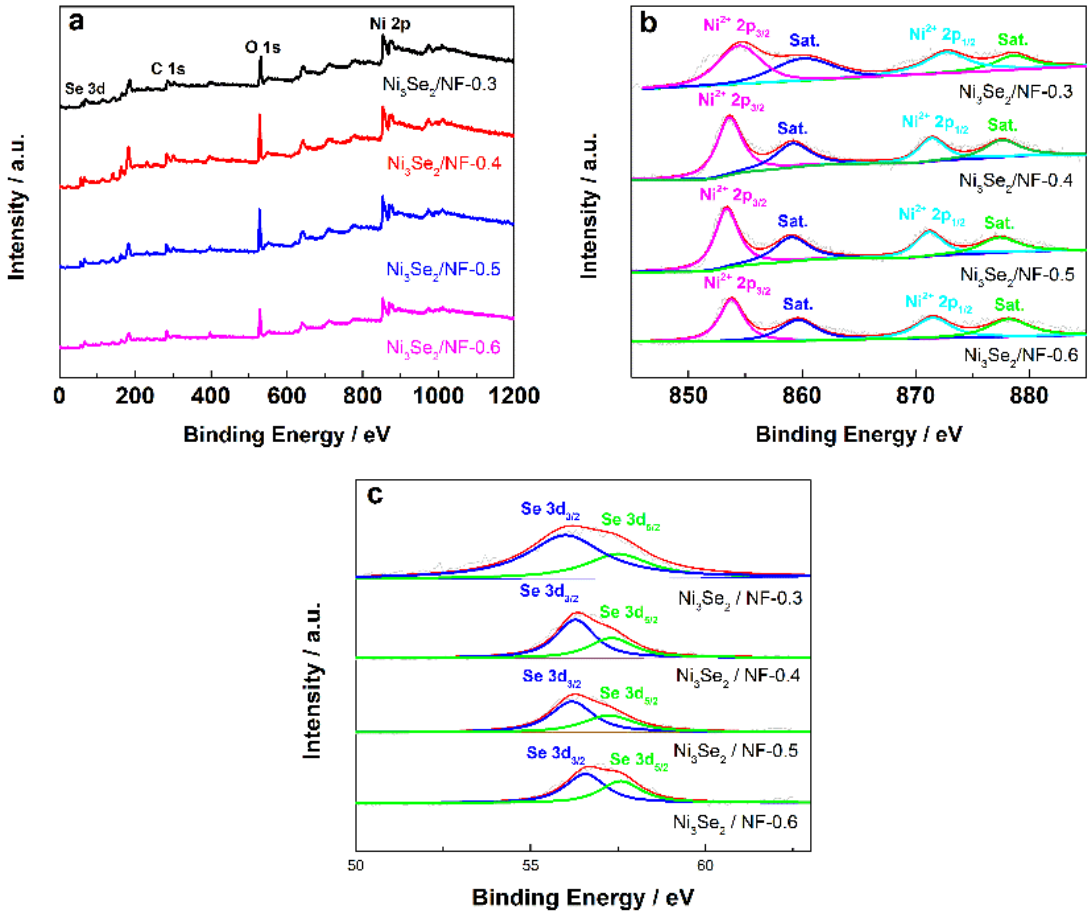

Figure S5. XPS of Ni_3Se_2/NF samples: (a) survey, (b) Ni 2p and (c) Se 3d

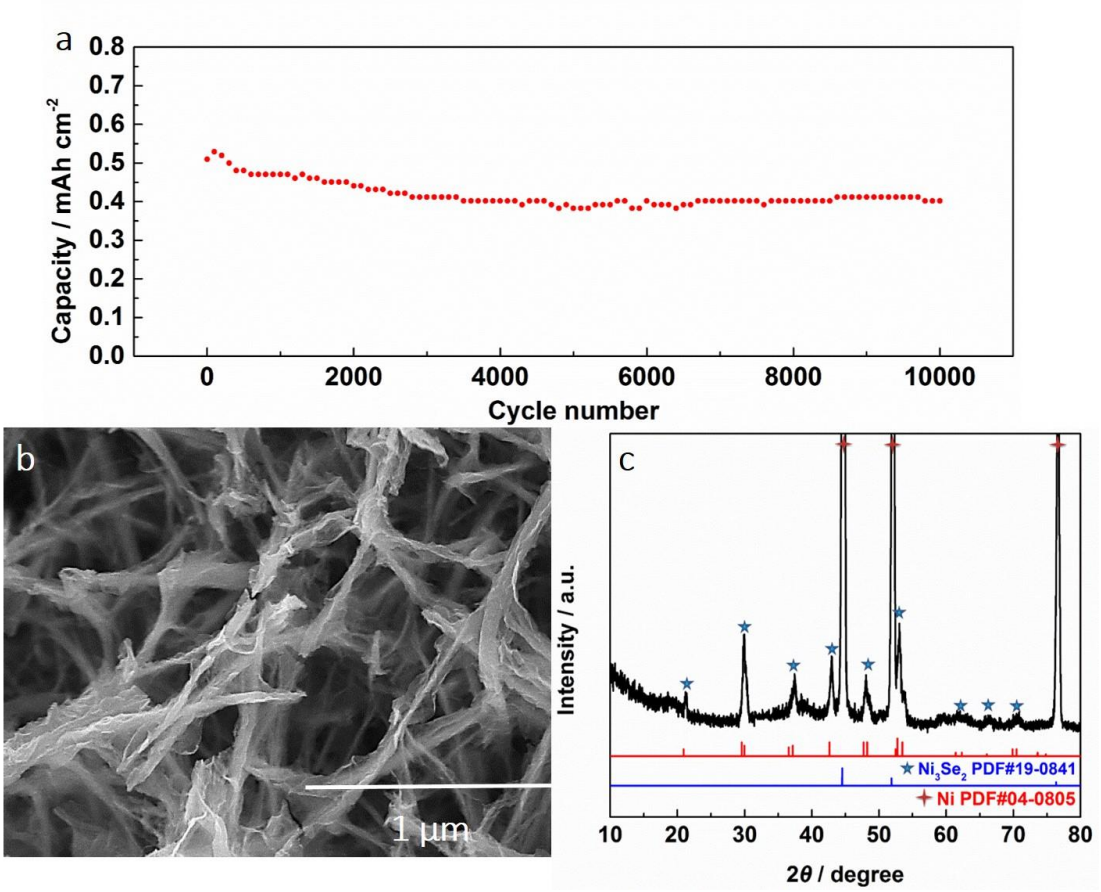

Figure S6. (a) Cycling stability of Ni_3Se_2/NF-0.4, (b) SEM and (c) XRD of Ni_3Se_2/NF-0.4 after stability cycling analysis.

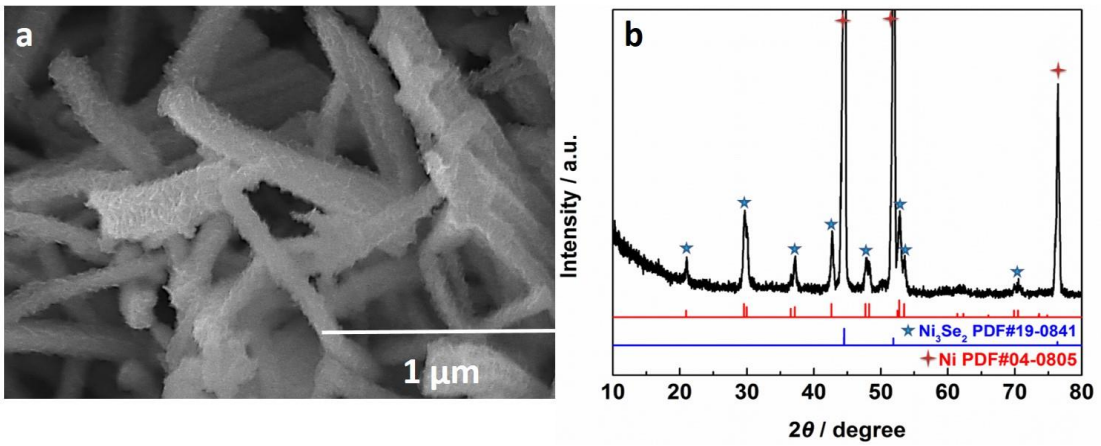

Figure S7. (a) SEM and (b) XRD of Ni_3Se_2/NF-0.4 after i-t curve analysis for HER.

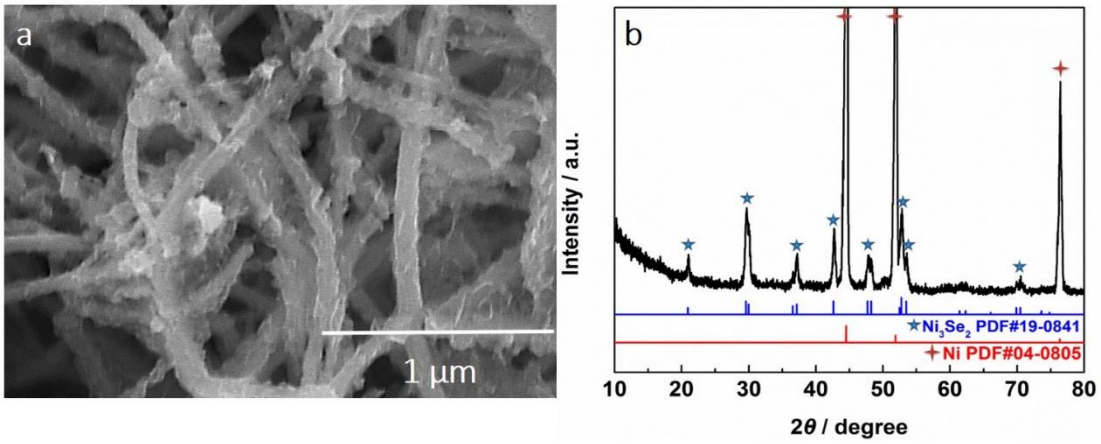

Figure S8. (a) SEM and (b) XRD of Ni_3Se_2/NF-0.4 after i-t curve analysis for OER.

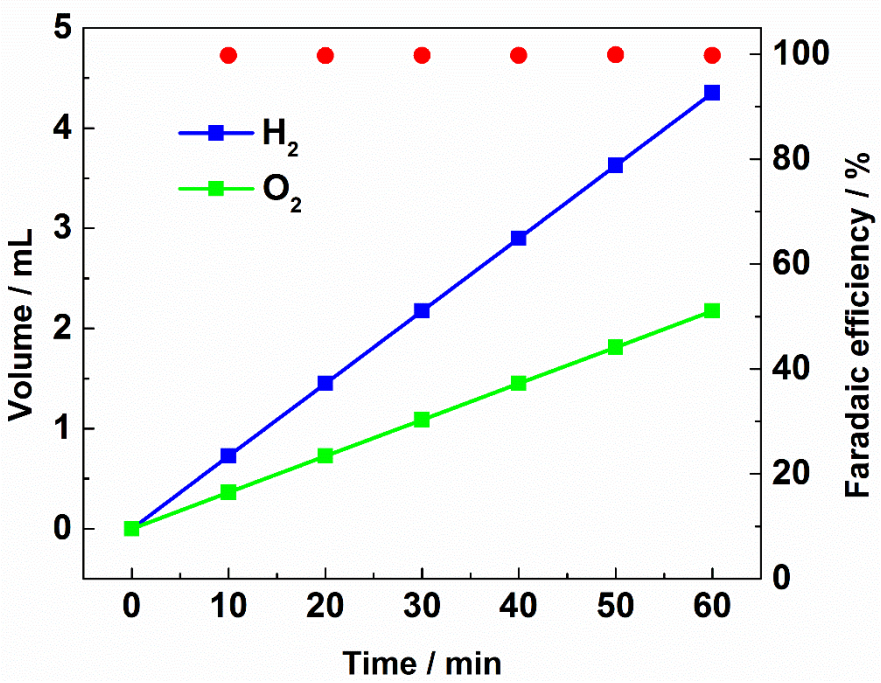

Figure S9. Gas volume versus time for the overall water splitting process.

Table S1. Mass loading of Ni_3Se_2/NF synthesized by different amounts of selenium powder

Electrode	Ni_3Se_2/NF-0.2	Ni_3Se_2/NF-0.3	Ni_3Se_2/NF-0.4	Ni_3Se_2/NF-0.5	Ni_3Se_2/NF-0.6
Mass loading / mg cm^{-2}	2.5	4.3	6.4	7.6	9.5

Table S2. XPS binding energy of Ni 2p and Se 3d of Ni_3Se_2/NF samples

Samples	Binding Energy / eV		Binding Energy / eV	
	Ni^{2+} $2P_{1/2}$	Ni^{2+} $2P_{3/2}$	Se $3d_{3/2}$	Se $3d_{5/2}$
Ni_3Se_2/NF-0.3	854.5	872.7	56	57.5
Ni_3Se_2/NF-0.4	853.6	871.4	56.2	57.3
Ni_3Se_2/NF-0.5	853.4	871.1	56.1	57.2
Ni_3Se_2/NF-0.6	853.7	871.5	56.5	57.6

Table S3. Benchmarking the capacitor performance of Ni_3Se_2/NF-0.4 against other nickel selenide-based materials in the alkaline electrolyte

Positive Electrode Materials	Negative Electrode Materials	Potential Window (V)	Energy Density (Wh kg^{-1})	Power Density (W kg^{-1})	References
Ni_3Se_2	AC	1.6	23.3	398.1	[1]
Ni_3Se_2	AC	1.5	32.8	677.03	[2]
CoSe	AC	1.5	18.6	750	[3]
$Ni_{0.67}Co_{0.33}Se$	RGO	1.5	36.7	750	[4]|
$Ni_{0.85}Se@MoSe_2$	AC	1.6	25.5	420	[5]
$NiSe@MoSe_2$	AC	1.65	27.5	400	[6]
Ni_3Se_2/NF	AC	1.6	42.6	284.8	This work

Table S4. Benchmarking the overpotential on Ni_3Se_2/NF-0.4 against other nickel selenide-based catalysts in alkaline electrolyte.

Catalysts	Electrolyte	η(HER, mV)/current density	Tafel Slope (mV dec^{-1})	η(OER) (mV)/current density	Tafel Slope (mV dec^{-1})	Cell Voltage for Two-Electrode Water Splitting (V) (10 mA cm^{-2})	References
Ni_3Se_2/NF	1 M KOH	---	---	315 (100 mA cm^{-2})	40.2	---	[7]
NiSe/NF	1 M KOH	---	---	411 (100 mA cm^{-2})	59.4	---	
$NiSe_x$/NF	1 M KOH	356 (100 mA cm^{-2})	96.5	303 (100 mA cm^{-2})	85.8	1.68	[8]
$NiSe_2$/Ti	1 M KOH	100 (10 mA cm^{-2})	107	370 (100 mA cm^{-2})	102	1.7	[9]
Co-Ni-Se/C/NF	1 M KOH	183 (100 mA cm^{-2})	81	300 (50 mA cm^{-2})	63	1.6	[10]
NF-Ni_3Se_2/Ni	1 M KOH	279 (100 mA cm^{-2})	79	353 (100 mA cm^{-2})	144	1.61	[11]
$(Ni,Co)_{0.85}Se$/NF	1 M KOH	169 (10 mA cm^{-2})	115.66	287 (20 mA cm^{-2})	86.75	1.65	[12]
NiSe/NF	1 M KOH	177 (10 mA cm^{-2})	58.2	290 (10 mA cm^{-2})	77.1	2.1	[13]
$Ni_{0.75}Se$/NF	1 M KOH	233 (10 mA cm^{-2})	86	360 (10 mA cm^{-2})	86	---	[14]
Ni_3Se_2/NF	1 M KOH	95 (50 mA cm^{-2})	67	320 (100 mA cm^{-2})	58	1.62 V	This work

Reference

1. S. Jiang, J. Wu, B. Ye, Y. Fan, J. Ge, Q. Guo and M. Huang, *J. Mater. Sci.- Mater. El.*, 2017, **29**, 4649-4657.
2. G. Nagaraju, S. M. Cha, S. C. Sekhar and J. S. Yu, *Adv. Energy Mater.*, 2017, **7**, 1601362.
3. Y. Zhu, Z. Huang, Z. Hu, L. Xi, X. Ji and Y. Liu, *Electrochim Acta*, 2018, **269**, 30-37.
4. H. Chen, S. Chen, M. Fan, C. Li, D. Chen, G. Tian and K. Shu, *J. Mater. Chem. A*, 2015, **3**, 23653-23659.
5. H. Peng, C. Wei, K. Wang, T. Meng, G. Ma, Z. Lei and X. Gong, *ACS appl. Mater. Interfaces*, 2017, **9**, 17067-17075.
6. H. Peng, J. Zhou, K. Sun, G. Ma, Z. Zhang, E. Feng and Z. Lei, *ACS Sustain Chem. Eng.*, 2017, **5**, 5951-5963.
7. A. Sivanantham and S. Shanmugam, *Appl. Catal. B - Environ.*, 2017, **203**, 485-493.
8. S. Dutta, A. Indra, Y. Feng, T. Song and U. Paik, *ACS appl. Mater. Interfaces*, 2017, **9**, 33766-33774.
9. T. Liu, A. M. Asiri and X. Sun, *Nanoscale*, 2016, **8**, 3911-3915.
10. F. Ming, H. Liang, H. Shi, X. Xu, G. Mei and Z. Wang, *J. Mater. Chem. A*, 2016, **4**, 15148-15155.
11. R. Xu, R. Wu, Y. Shi, J. Zhang and B. Zhang, *Nano Energy*, 2016, **24**, 103-110.
12. K. Xiao, L. Zhou, M. Shao and M. Wei, *J. Mater. Chem. A*, 2018, **6**, 7585-7591.
13. H. Wu, X. Lu, G. Zheng and G. W. Ho, *Adv. Energy Mater.*, 2018, **8**, 1702704.
14. D. Yang, T. Sano, H. Sasabe, L. Yang, S. Ohisa, Y. Chen, Y. Huang and J. Kido, *ACS appl. Mater. Interfaces*, 2018, **10**, 26465-26472.