Electronic Supplementary Information for:

Sulfur Vacancies Promoting Fe-Doped Ni_3S_2 Nanopyramid Arrays as Efficient Bifunctional Electrocatalysts for Overall Water Splitting

Shu-Chao Sun[a,b], Fei-Xiang Ma[a,b], Yang Li[a,b], Li-Wei Dong[c], Huan Liu[a,b], Chun-Ming Jiang[a,b], Bo Song[d], Liang Zhen[*,a,b], Cheng-Yan Xu[*,a,b,e]

[a] School of Materials Science and Engineering, Harbin Institute of Technology, Harbin 150001, China

[b] MOE Key Laboratory of Micro-Systems and Micro-Structures Manufacturing, Harbin Institute of Technology, Harbin 150080, China

[c] School of Environmental and Material Engineering, Yantai University, Yantai 264005, China

[d] Centre for Composite Materials and Structures, Harbin Institute of Technology, Harbin 150080, China

[e] School of Materials Science and Engineering, Harbin Institute of Technology (Shenzhen), Shenzhen 518055, China

Corresponding authors: lzhen@hit.edu.cn (L.Z.), cy_xu@hit.edu.cn (C.-Y.X.)

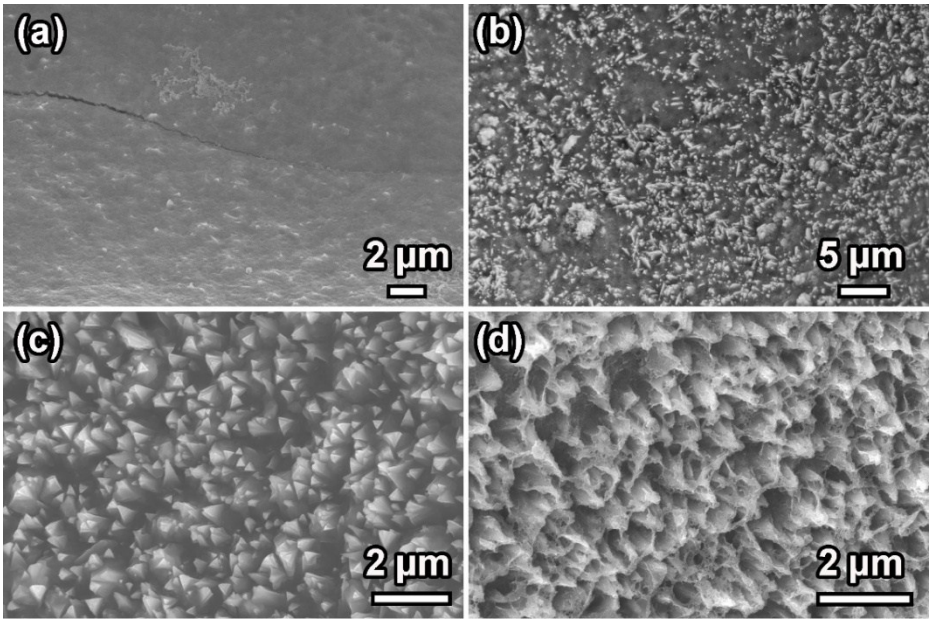

Fig. S1. SEM images of pristine and Fe-doped Ni_3S_2. (a) Pristine Ni_3S_2; (b) Fe-doped Ni_3S_2, 0.10 mmol; (c) Fe-doped Ni_3S_2, 0.15 mmol; (d) Fe-doped Ni_3S_2, 0.20 mmol.

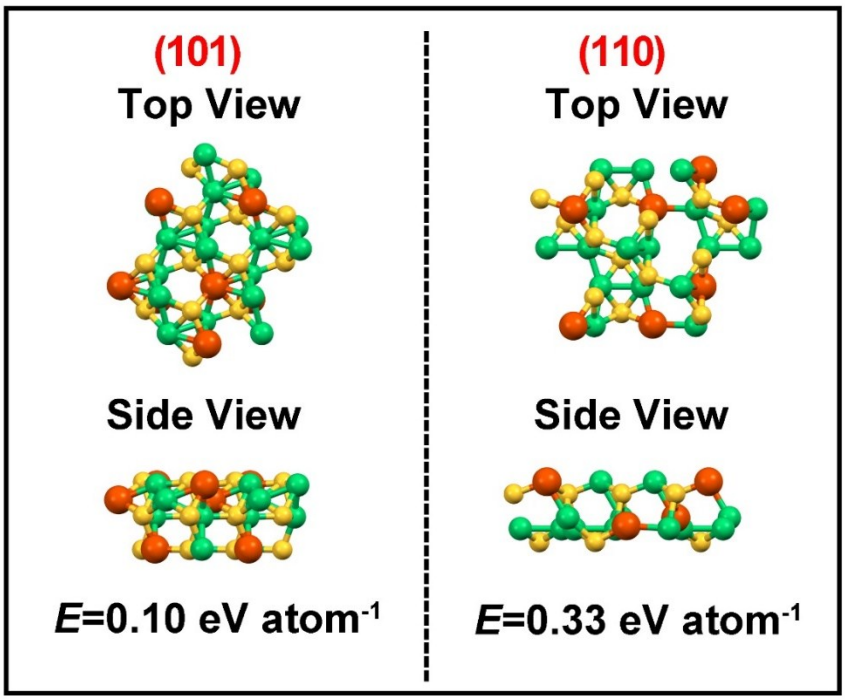

Fig. S2. Top and side view of (101) and (110) facet models for S_V-Fe-Ni_3S_2 and their calculated surface energy.

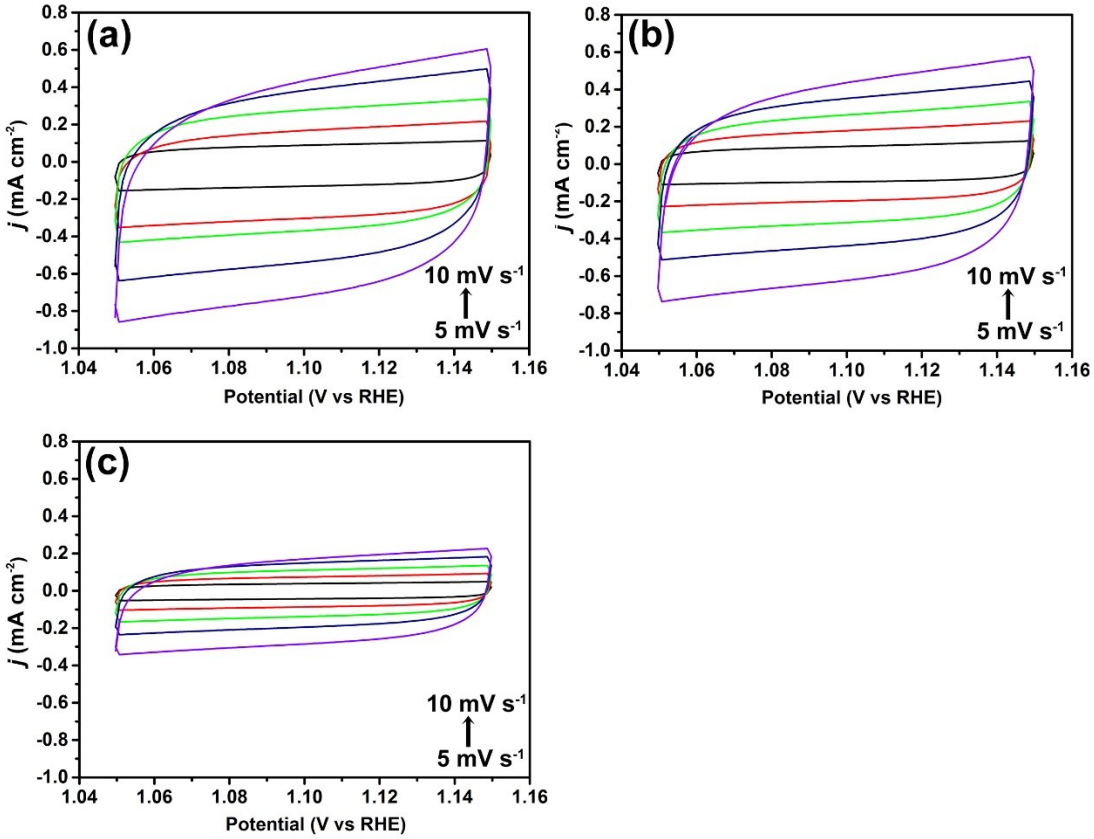

Fig. S3. Cyclic voltammograms of (a) S_V-Fe-Ni_3S_2, (b) Fe-Ni_3S_2 and (c) Ni_3S_2 in the non-Faradaic capacitance current range at scan rates of 10, 20, 30, 40, and 50 mV s^{-1}.

Table S1. Comparison of the catalytic performance for OER in 1 M KOH between S_V-Fe-Ni_3S_2 nanopyramid arrays and other Ni_3S_2-based electrocatalysts in the literature.

	η @ 10 mA cm^{-2} (mV)	η @ 100 mA cm^{-2} (mV)	Tafel slope (mV dec^{-1})	Refs.
$Fe_{11.8\%}$-Ni_3S_2/NF	–	253	65.5	1
Fe-Ni_3S_2/FeNi	282	–	54	2
$Fe_{0.1}$-NiS_2 NA/Ti	–	231	43	3
$Fe_{17.5\%}$-Ni_3S_2	214	249	42	4
Ni_3S_2 nanorod array	217	–	163	5
MoS_2/Ni_3S_2	218	290	88	6
Ni_3S_2/MnS	228	–	46	7
3D coral-like Ni_3S	242	318	103	8
High-index faceted Ni_3S_2	260	–	–	9
Ni_3S_2/MnO_2	260	348	61	10
N-doped Ni_3S_2	284.7	–	–	11
$Ni_xCo_{3-x}S_4$/Ni_3S_2/NF	160	320	95	12
S_V-Fe-Ni_3S_2 NP/NF	171	245	49	this work

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