

Electronic Supplementary Information (ESI)

Perovskite decorated with oxygen vacancies and Fe-Ni alloy nanoparticles as high-efficiency electrocatalyst for oxygen evolution reaction

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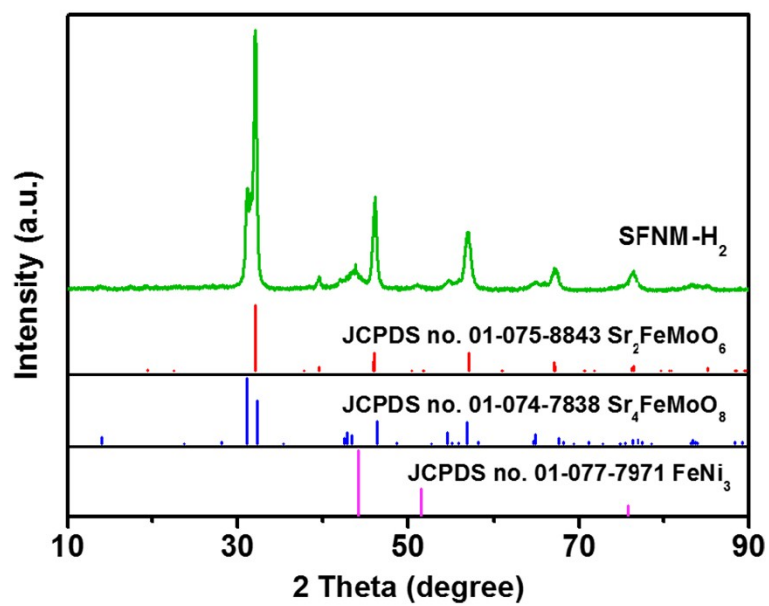


Fig. S1 Powder X-ray diffraction patterns of SFNM-H₂.

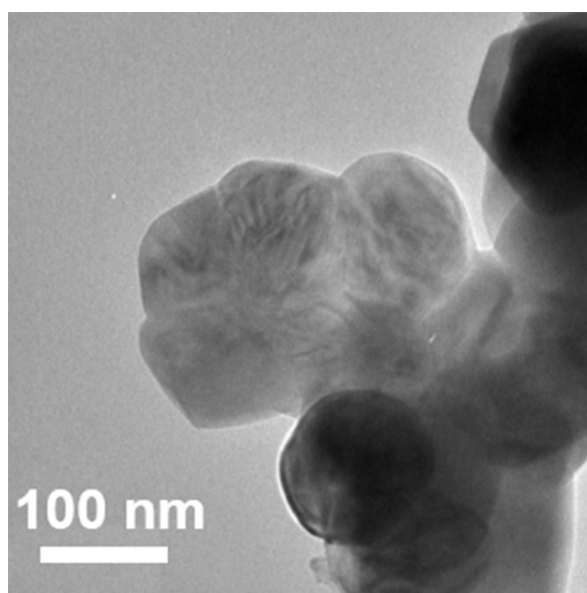


Fig. S2 TEM image of SFNM.

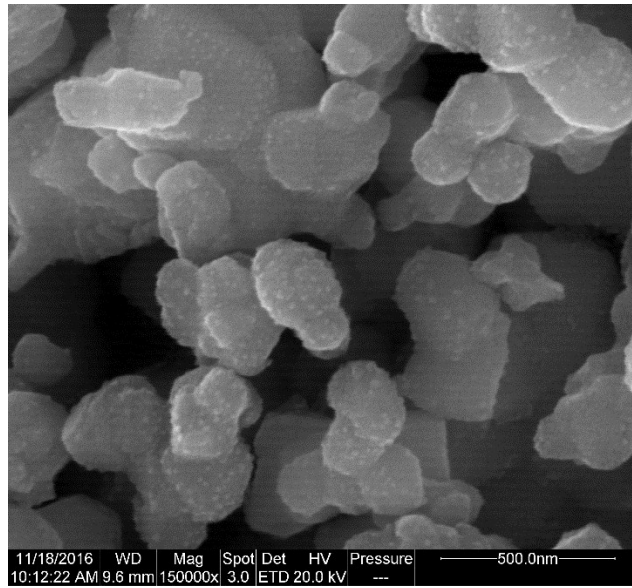


Fig. S3 SEM image of SFNM-5% H_2 /Ar.

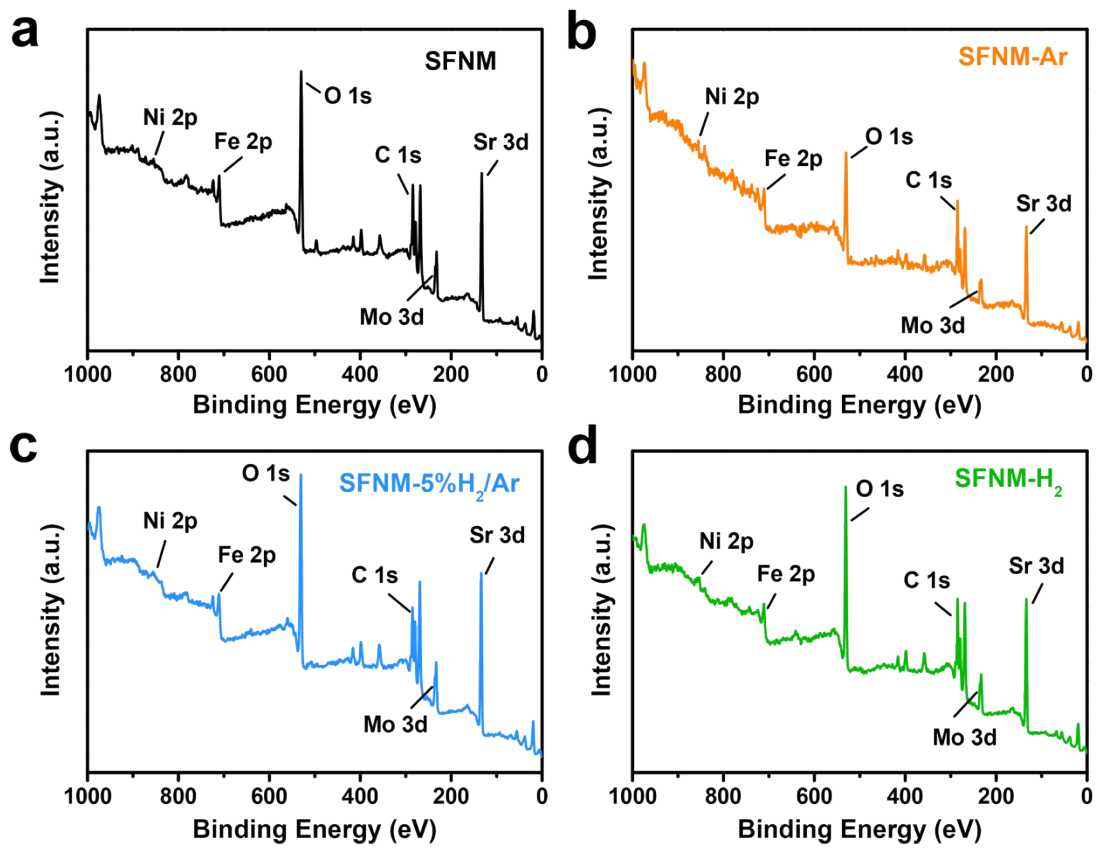


Fig. S4 XPS survey spectra of SFNM, SFNM-Ar, SFNM-5% H_2 /Ar and SFNM- H_2 .

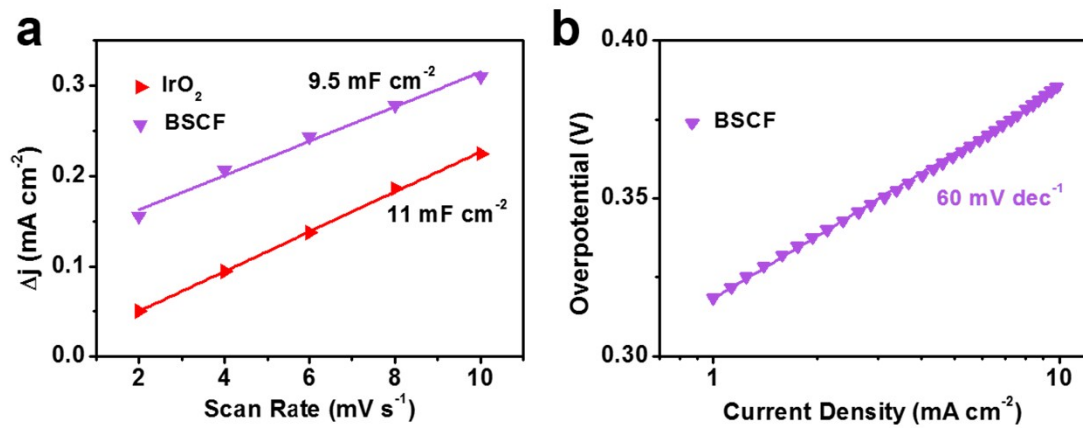


Fig. S5 (a) Charging current density differences Δj plotted against scan rates of IrO₂ and BSCF. (b) Tafel plots of BSCF.

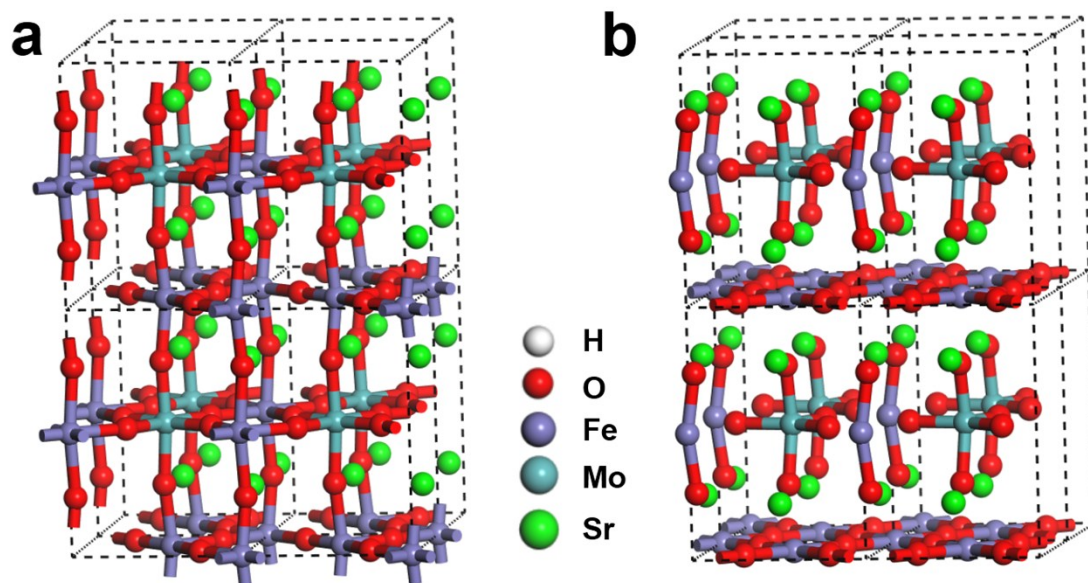


Fig. S6 Geometries of SFM with oxygen vacancies near Fe sites (a) and near Mo sites (b), respectively. When there are oxygen vacancies near Mo sites, the structure of SFM perovskite falls apart indicating oxygen vacancies are less prone to appear near Mo site.

Table S1. Ni 2p_{3/2} XPS fitting data for SFNM, SFNM-Ar, SFNM-5%H₂/Ar and SFNM-H₂. The unit of binding energies is eV.

catalysts	Ni ⁰	Ni ²⁺	Ni ³⁺	S1 ^[a]
SFNM		855.0	856.5	861.6
SFNM-Ar		855.0		862.3
SFNM-5%H ₂ /Ar	852.2	854.9		861.4
SFNM-H ₂	852.2	854.9		860.7

^[a]S1 is the satellite peak of Ni 2p_{3/2}.

Table S2. Fe 2p XPS fitting data for SFNM, SFNM-Ar, SFNM-5%H₂/Ar and SFNM-H₂. The unit of binding energies is eV.

catalysts	Fe 2p _{3/2}					Fe 2p _{1/2}				
	Fe ⁰	Fe ²⁺	Fe ³⁺	Fe ⁴⁺	S2 ^[b]	Fe ⁰	Fe ²⁺	Fe ³⁺	Fe ⁴⁺	S3 ^[b]
SFNM		709.	710.	713.	718.		722.	724.	726.	731.
		4	6	4	5		9	3	8	4
SFNM-Ar		709.	710.		718.		722.	724.		731.
		3	6		5		9	3		4
SFNM-5%H ₂ /Ar	706.	709.	710.		716.	720.	722.	724.		731.
	8	3	6		8	1	9	3		3
SFNM-H ₂	706.	709.	710.		716.	720.	722.	724.		731.
	8	3	7		0	0	9	3		2

^[b]S2 and S3 are the satellite peaks of Ni 2p_{3/2} and Ni 2p_{1/2}, respectively.

Note: From XPS spectra of Ni and Fe, the atomic ratios of Fe⁰ and Ni⁰ in SFNM-5%H₂/Ar and SFNM-H₂ are 1.02 and 1.31, respectively. The ratios of Ni⁰:(Ni⁰+Ni²⁺) in SFNM-5%H₂/Ar and SFNM-H₂ is 0.23 and 0.31, respectively. The ratios of Fe⁰:(Fe⁰+Fe²⁺+Fe³⁺) in SFNM-5%H₂/Ar and SFNM-H₂ are 0.03 and 0.12, respectively. Although XPS obtains the surface information, the XPS results can also reflect that Ni-Fe alloy nanoparticles of SFNM-5%H₂/Ar should be less than those of SFNM-H₂, in accord with the results from XRD, SEM, HRTEM and Mapping.

Table S3. Mo 3d XPS fitting data for SFNM, SFNM-Ar, SFNM-5%H₂/Ar and SFNM-H₂. The unit of binding energies is eV.

catalysts	Mo 3d _{5/2}		Mo 3d _{3/2}	
	Mo ⁵⁺	Mo ⁶⁺	Mo ⁵⁺	Mo ⁶⁺
SFNM		232.3		235.4
SFNM-Ar		232.3		235.5
SFNM-5%H ₂ /Ar	231.3	232.4	234.6	235.6
SFNM-H ₂	231.4	232.4	234.7	235.6

Table S4. O 1s XPS fitting data for SFNM, SFNM-Ar, SFNM-5%H₂/Ar and SFNM-H₂. The unit of binding energies is eV.

catalysts	O _{lattice}	O _{ad}
SFNM	529.08	531.36
SFNM-Ar	529.14	531.36
SFNM-5%H ₂ /Ar	529.24	531.36
SFNM-H ₂	529.30	531.11