

**Supporting Information for**  
**Mo doping and Se vacancy engineering for boosting electrocatalytic**  
**water oxidation by regulating the electronic structure of self-**  
**supported Co<sub>9</sub>Se<sub>8</sub>@NiSe**

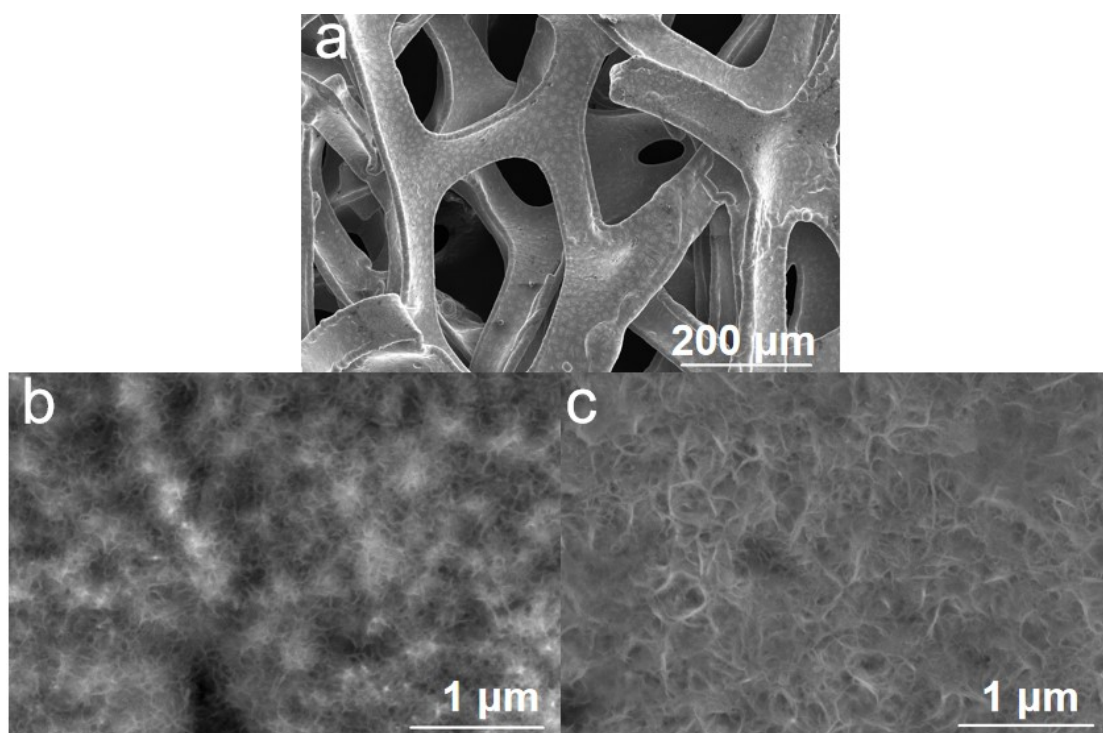
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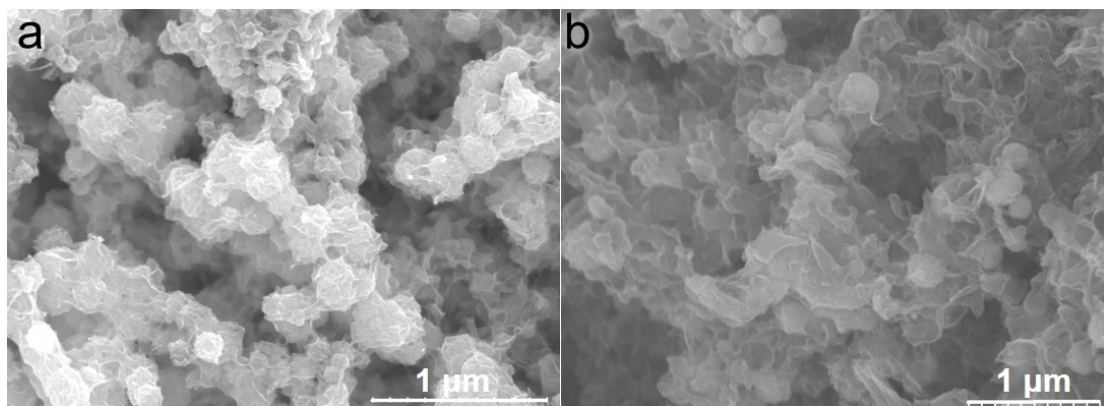
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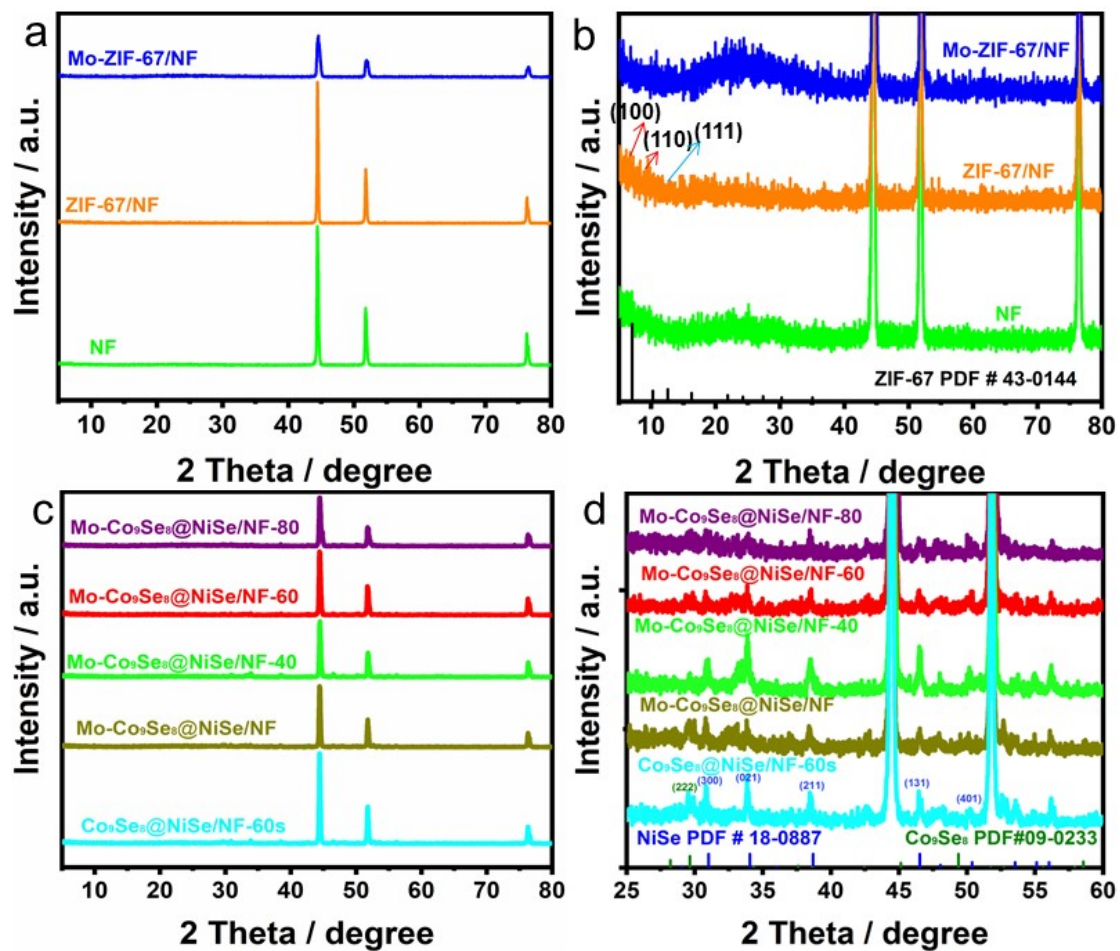
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**Fig.S1** (a) SEM images of (a) pre-treated nickel foam, (b) Mo-Co<sub>9</sub>Se<sub>8</sub>@NiSe/NF-40, (c) Mo-Co<sub>9</sub>Se<sub>8</sub>@NiSe/NF-80.



**Fig.S2** SEM images of (a) Mo-Co<sub>9</sub>Se<sub>8</sub>@NiSe/NF, (b) Co<sub>9</sub>Se<sub>8</sub>@NiSe/NF-60.



**Fig.S3** (a) XRD patterns of pre-treated NF, ZIF-67/NF, Mo-ZIF-67/NF, and (b) their corresponding locally enlarged XRD patterns. (c) XRD patterns of Mo-Co<sub>9</sub>Se<sub>8</sub>@NiSe/NF-40, Mo-Co<sub>9</sub>Se<sub>8</sub>@NiSe/NF-60, Mo-Co<sub>9</sub>Se<sub>8</sub>@NiSe/NF-80, Mo-Co<sub>9</sub>Se<sub>8</sub>@NiSe/NF, Co<sub>9</sub>Se<sub>8</sub>@NiSe/NF-40, and (d) their corresponding locally enlarged XRD patterns.

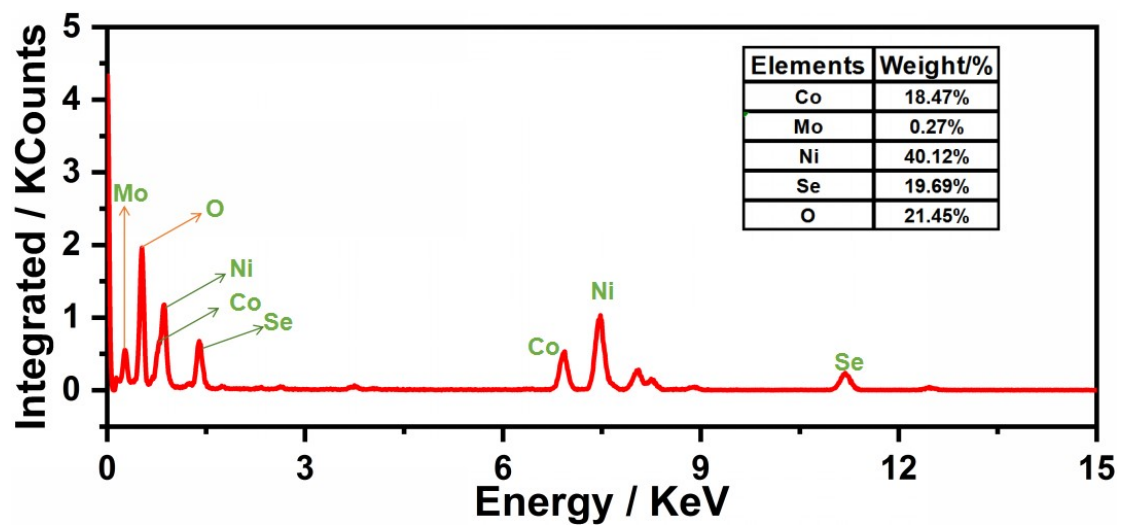


Fig.S4 EDS spectrum of Mo-Co<sub>9</sub>Se<sub>8</sub>@NiSe/NF-60.

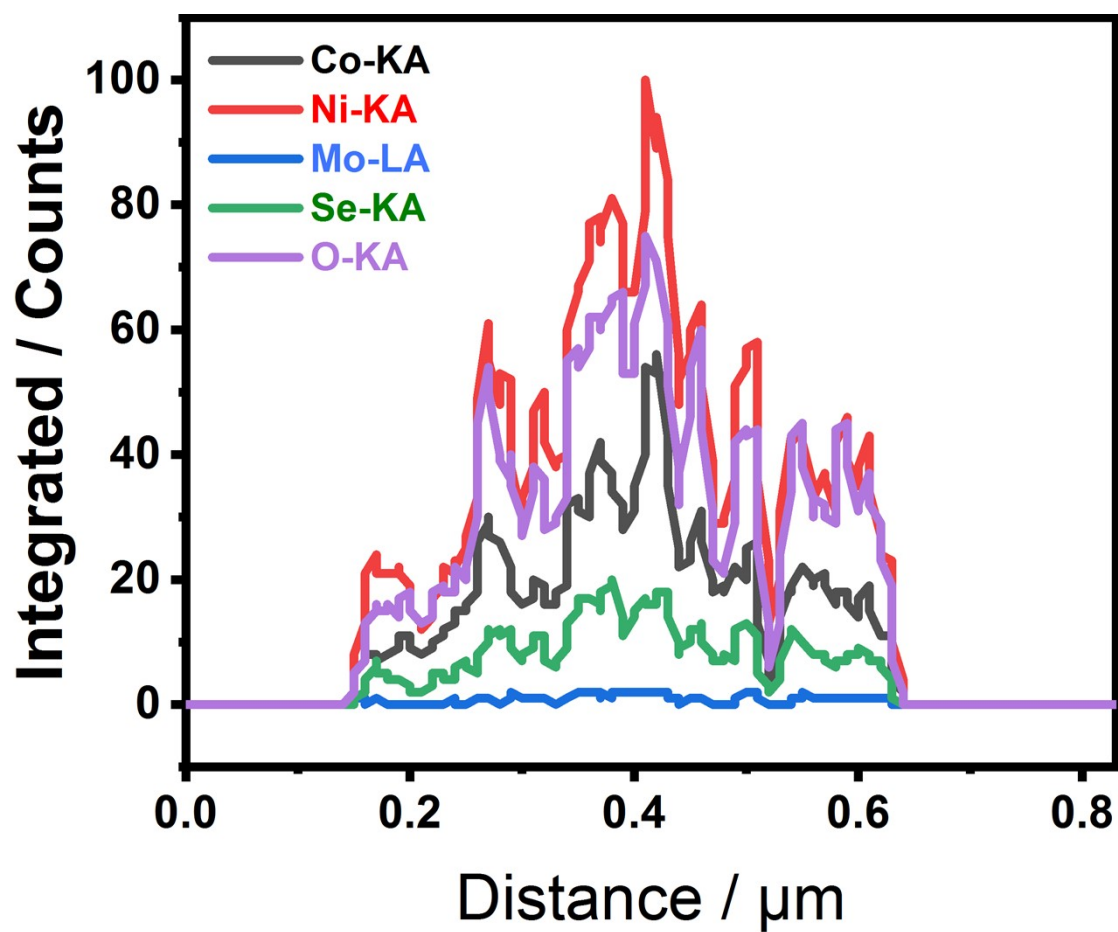
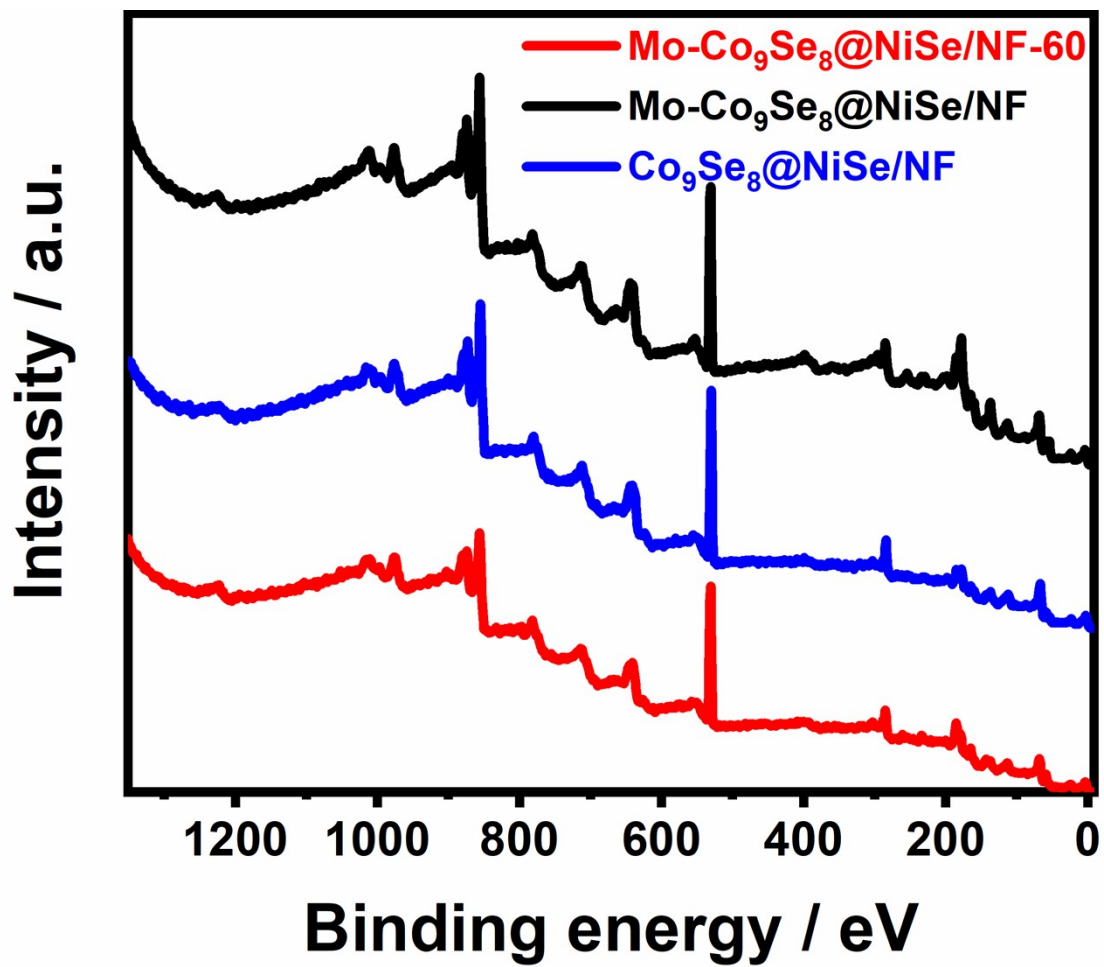
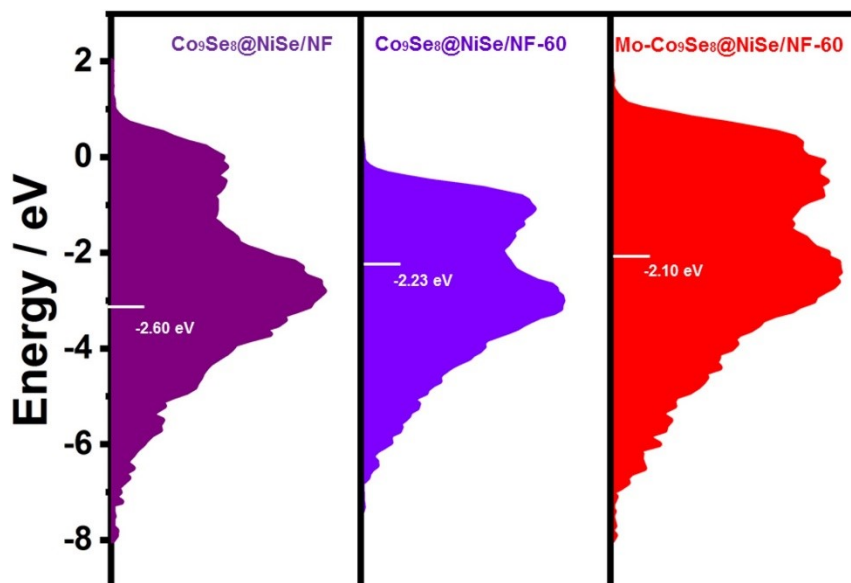


Fig.S5 Line-scan profile of Mo-Co<sub>9</sub>Se<sub>8</sub>@NiSe/NF-60.

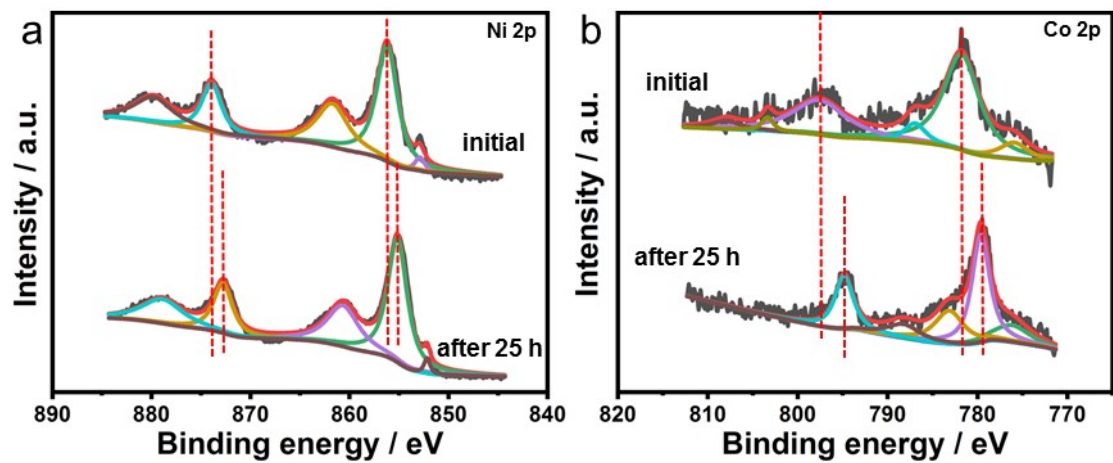


**Fig.S6** Survey spectrum of Mo-Co<sub>9</sub>Se<sub>8</sub>@NiSe/NF-60, Mo-Co<sub>9</sub>Se<sub>8</sub>@NiSe/NF, Co<sub>9</sub>Se<sub>8</sub>@NiSe/NF-60.

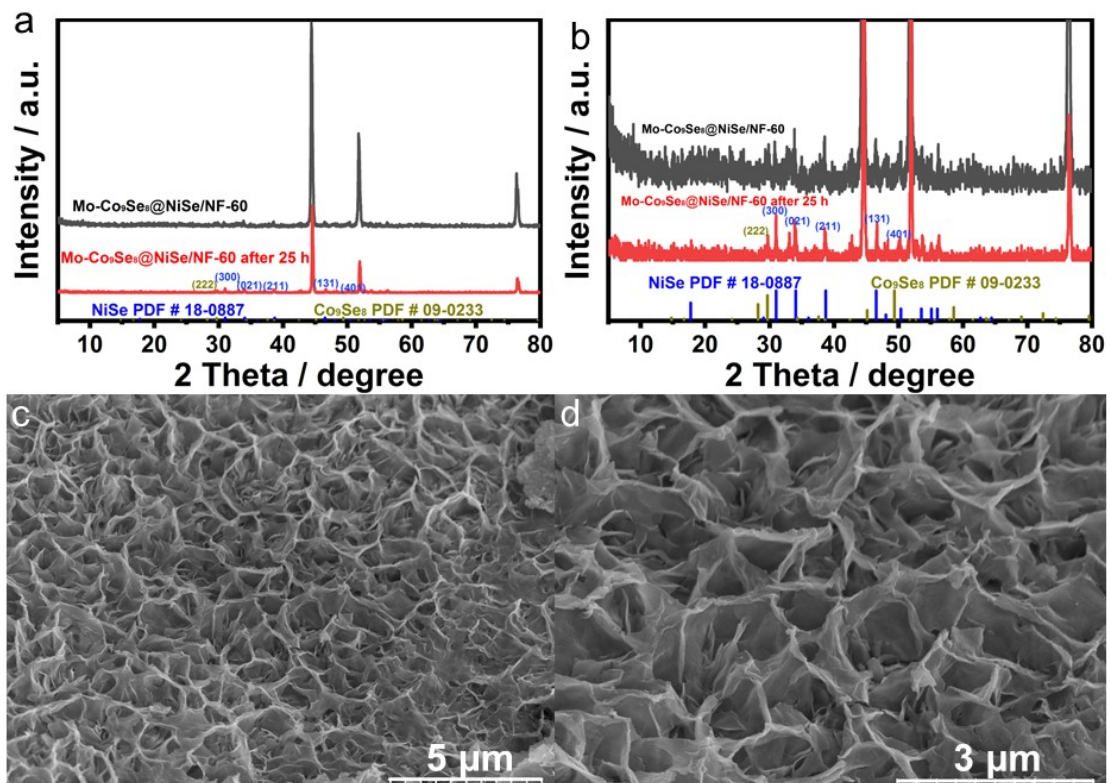


**Fig.S7** Surface valence band spectra and the calculated d-band centers of Co<sub>9</sub>Se<sub>8</sub>@NiSe/NF, Co<sub>9</sub>Se<sub>8</sub>@NiSe/NF-60, and Mo-Co<sub>9</sub>Se<sub>8</sub>@NiSe/NF-60.





**Fig.S8** The high-resolution XPS spectra of (a) Co 2p and (b) Ni 2p before and after CP tests.



**Fig.S9** (a) XRD pattern of Mo-Co<sub>9</sub>Se<sub>8</sub>@NiSe/NF-60 before and after CP tests and (b) corresponding locally enlarged pattern. (c, d) SEM images of Mo-Co<sub>9</sub>Se<sub>8</sub>@NiSe/NF-60 with different magnification.