Supplementary Information (SI) for CrystEngComm
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Supporting Information

Highly Efficient Overall Water Splitting Enabled by a Bimetallic FeRu-MOF Electrocatalyst

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Density Functional Theory (DFT) Calculations

All spin-polarized density functional theory (DFT) calculations were conducted utilizing the Vienna Ab initio Simulation Package (VASP) [1]. To depict ion-electron interactions, the projector augmented wave (PAW) method[2] along with pseudopotentials were adopted, while electron-electron interactions were addressed using the Perdew-Burke-Ernzerhof (PBE)[3] generalized gradient approximation (GGA).

A vacuum layer with a thickness of 20 Å was introduced above the slab surface. Subsequently, structural optimization was carried out with relaxed lattice parameters for the slab configuration. Spin polarization was incorporated into all calculations, employing a 2×3×1 k-point mesh and a plane-wave cutoff energy of 500 eV. The energy convergence criterion was set at 1×10^{-5} eV, and the force convergence threshold was established as 0.05 eV/Å.

The Van der Waals interaction was accounted for using the DFT-D3BJ method[4]. For structural visualization, VESTA[5] was employed, and post-processing was performed using the vaspkit toolkit[6].

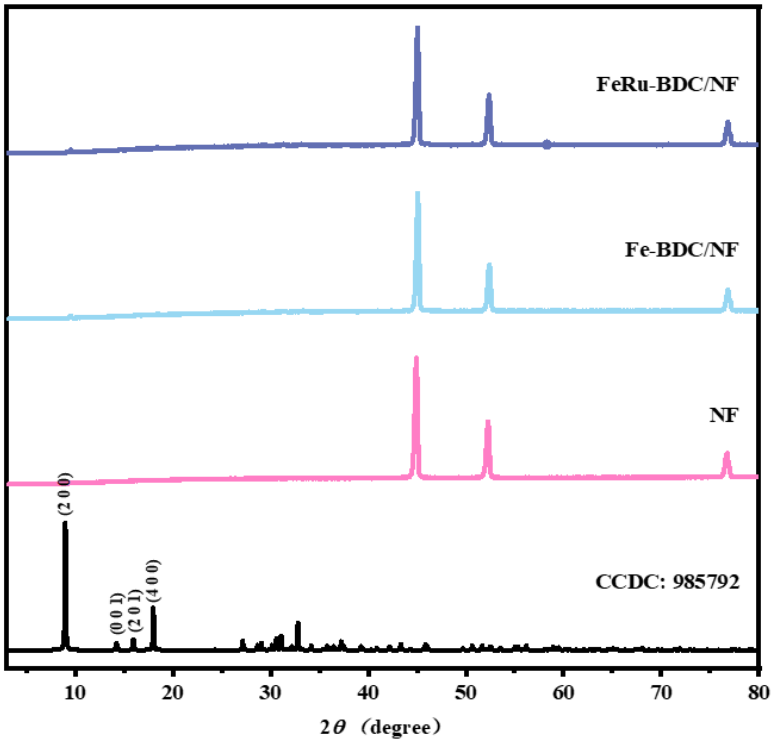

Fig. S1 The PXRD pattern of FeRu-BDC/NF material.

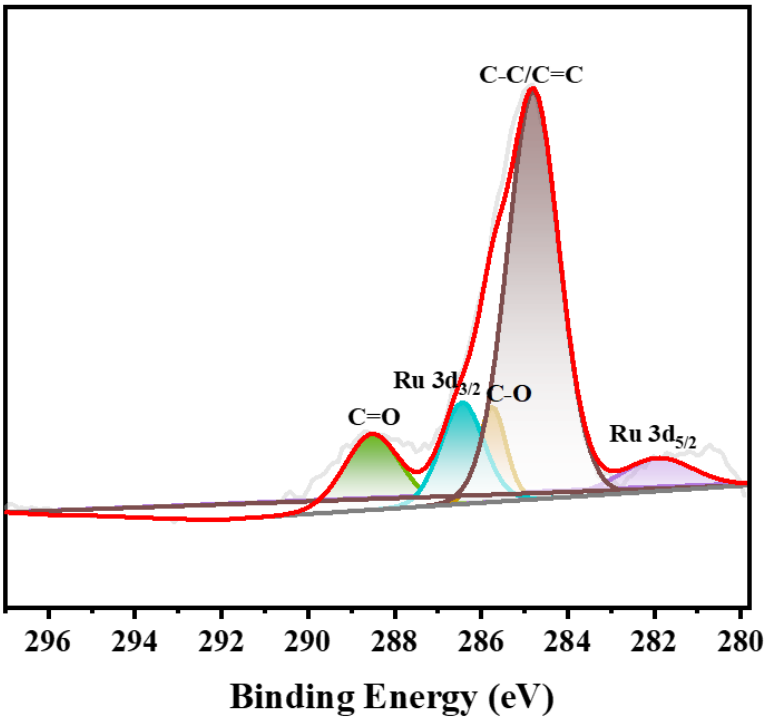

Fig. S2 High-resolution XPS spectra of C 1s for FeRu-BDC/NF.

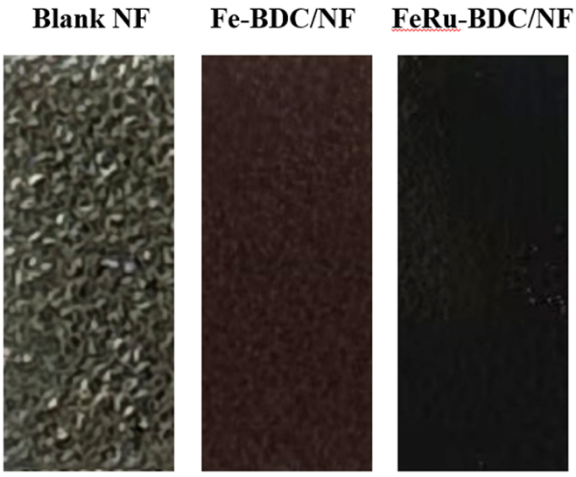

Fig. S3 The color change of the foam nickel during the synthesis process

Table S1. HER comparison in 1.0 M KOH with the recently reported literatures.

Materials	η_{10}**/mV**	**Reference**
FeRu-BDC/NF	54	**This work**
FeNi-MOF@NiMo-LDH	160	[7]
Ru-FeMn-MOF	86	[8]
0.04 Ru/FeCo-MOF	180	[9]
$FeMn_6Ce_{0.5}$-MOF-74/NF	186	[10]
Mn-MOF/NF	125	[11]
CdFe-MOF	148	[12]
Fe-MOF/Au-8/FF	130	[13]
$VeNi_{0.06}Fe_{0.06}$MOF/GO	90	[14]
$FeS_{2-x}Se_x$/CoS@CC	285.2	[15]

Table S2. OER comparison in 1.0 M KOH with the recently reported literatures.

Materials	η_{50}/**mV**	**Reference**
FeRu-BDC/NF	230	**This work**
Ru/FeCo-MOF	309	[9]
$FeS_{2-x}Se_x$/CoS@CC	357.8	[15]
NiFeMo-MOF/NF	239	[16]
Fe@Co-MOF-3	248	[17]
Fe-MOF/NF	240	[18]
$Fe_{0.1}$-Ni-MOF/NF	243	[19]
$Co_{0.75}Fe_{0.25}$-MOF	257	[20]
V-Ni MOF@FeOOH	267@20	[21]
Ru@NiCo-MOF HPNs	78.8@10	[22]

Table S3. Summary of overall water-splitting electrocatalysts.

Materials	**Voltage/mV**	**Reference**
FeRu-BDC/NF	1.47	**This work**
FeNi-MOF@NiMo-LDH	1.62	[7]
CdFe-MOF	1.68	[12]
Fe-MOF/Au-8/FF	1.61	[13]
NiFeMo-MOF/NF	1.50	[16]
Ru@NiCo-MOF-4||Pt/C	1.57	[22]
NiRu-PTA/NF	1.54	[23]
$FeNi_3S_2$@NiFe-MOF/NF	1.6	[24]
Ce@NiFe-MOF-5	1.56	[25]
CoFe-MS/MOF	1.54	[26]
Ru/$NiFe(OH)_x$/NiFe-MOF||Pt/C	1.54	[27]

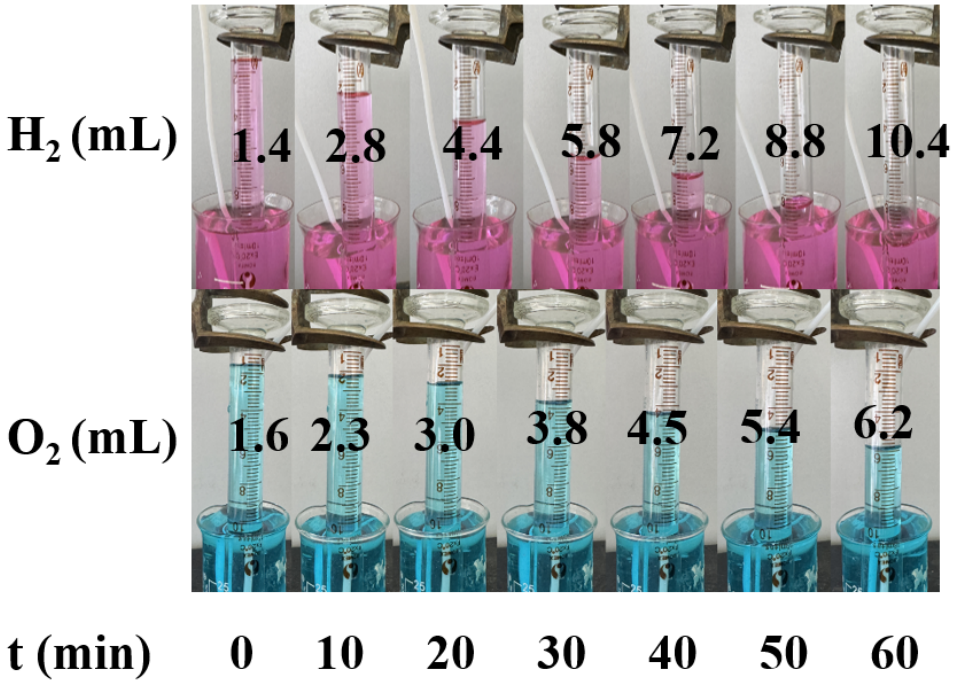

Fig. S4 Faraday efficiency measured using the drainage setup. H_2 and O_2 gas volumes were collected at 0 min, 10 min, 20 min, 30 min, 40 min, 50 min, and 60 min.

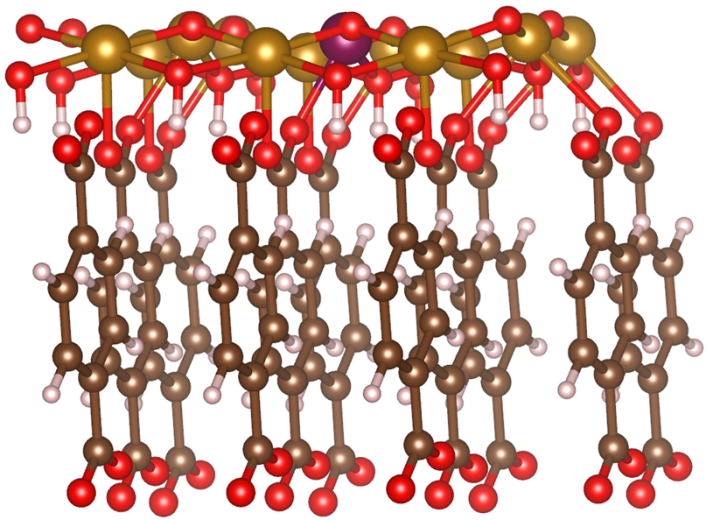

Fig. S5 Schematic model of FeRu-BDC

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