Defect-Enriched Iron Fluoride-Oxide Nanoporous Thin Films Bifunctional Catalyst for Water Splitting
Xiujun et al.
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Supplementary Figure 22 | STEM characterization of IFONFs-45. a,b STEM images of IFONFs fluorinated with 60 min. Scale bar, a,b 5 nm.
Supplementary Figure 23 | STEM characterizations of IFONFs fluorinated with 90 min. a,b
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Supplementary Figure 28 | Capacitance measurements. Cyclic voltammograms and capacitive currents plotted as a function of scan rate in 1 M KOH at scan rates of 10, 20, 40, 60, 80, 100, 120, 140, 160, 180, and 200 mV s⁻¹ for a-b the raw Fe-oxide PTF and IFONFs prepared with various time, c-d 15 min, e-f 30 min, g-h 45 min, i-j 60 min, and k-l 90 min, respectively, where no obvious electrochemical features corresponding to the Faradic current are observed.
Supplementary Figure 29 | CV curves and ECSA of Fe$_2$O$_3$ and FeF$_2$ PTF. Cyclic voltammograms and capacitive currents plotted as a function of scan rate in 1 M KOH at scan rates of 10, 20, 40, 60, 80, 100, 120, 140, 160, 180, and 200 mV s$^{-1}$ for a-b Fe$_2$O$_3$ PTF; c-d FeF$_2$ PTF.
Supplementary Figure 30 | CVs of IFONFs-45 and Pt/C. CVs of IFONFs-45 and Pt/C in 1 M KOH (pH 14) with a scan rate of 50 mV s$^{-1}$ in the region of $-0.2$ to $0.6$ V vs RHE.
Supplementary Figure 31 | Stability test of Pt/C. Time-dependent current density curve of Pt/C at a fixed overpotential of -70 mV to drive 82 mA cm$^{-2}$ for 30000 s in 1 M KOH.
Supplementary Figure 32 | STEM characterizations of IFONFs-45 electrode. a,b STEM images of IFONFs-45 after 3000 cycles HER testing. Scale bar, a,b 5 nm.
Supplementary Figure 33 | Tafel slopes of RuO$_2$, Fe-oxide and IFONFs hybrid catalysts.
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Supplementary Figure 36 | Calculation for the number of active sites. a, c, e, g, I and k Cyclic voltammograms of Fe-oxide PTF and IFONFs hybrids under different scan rates increasing from 10 to 100 mV s$^{-1}$ in 1 M KOH. b, d, f, h, j and l Linear relationship of the peak current for the oxidation wave at the scan rate.
Supplementary Figure 37 | Impedance studies of Fe-oxide PTF and IFONFs. a EIS data for Fe-oxide PTF and IFONFs hybrids in 1 M KOH under OER overpotential of 500 mV, b the enlargement of area denoted by dash squares in a, c the equivalent circuit model for the impedance spectroscopy.
Supplementary Figure 38 | XPS spectra of IFONFs-45 before and after OER durability test.
High-resolution XPS in the a Fe 2p, b O 1s, and c F 1s regions of IFONFs-45 before and after 100000 s OER durability test.
Supplementary Figure 39 | Chemical stability of IFONFs-45 electrode. LSV curves of IFONFs-45 electrode before (red curve) and after stored under ambient conditions for one year and four months (black dash curve) for a HER and b OER, respectively. c,d HRTEM images for IFONFs-45 stored under ambient conditions for one year and four months. Scale bar, c,d 5 nm.
Supplementary Figure 40 | Water splitting performance characterization. a Polarization curves of IFONFs-45 (±), Pt/C (+)/Pt/C (−), and Ir/C (+)/Pt/C (−) for overall water splitting in a two-electrode configuration (not iR-corrected). b Chronopotentiometry curves of IFONFs-45 and Ir/C (+)/Pt/C (−) under a current density of 10 mA cm$^{-2}$ without iR correction. All experiments were carried out in 1 M KOH.
**Supplementary Figure 41** | Faradic efficiencies calculations for both HER and OER. 

**a** Image showing the evolution of H$_2$ and O$_2$ gas on IFONFs-45 in a well-sealed H-type cell. The IFONFs-45 samples are sealed with parafilm using electric wires connected with electrochemical workstation. 

**b** Experimental and theoretical amounts of H$_2$ and O$_2$ by the IFONFs-45 electrode at a fixed current density of 40 mA cm$^2$. 
Supplementary Table 1. Fe content determined by ICP-MS and quantitative surface analysis by XPS.

| Samples      | Fe loading (wt%) | Surface atomic concentration (at%) |
|--------------|------------------|-----------------------------------|
|              |                  | C  | O  | F  | Fe  |
| Fe-oxide     | 21.5             | 37.17 | 45.62 | - | 17.21 |
| IFONFs-15    | 19.3             | 35.76 | 39.85 | 6.76 | 17.63 |
| IFONFs-30    | 19.2             | 36.10 | 37.51 | 9.34 | 17.05 |
| IFONFs-45    | 18.8             | 35.42 | 33.76 | 12.45 | 18.37 |
| IFONFs-60    | 18.6             | 35.30 | 33.17 | 14.26 | 17.27 |
| IFONFs-90    | 14.8             | 35.42 | 30.38 | 16.32 | 17.88 |

Fe-oxide PTF has a higher Fe content of 21.5 at% derived from the ICP-MS measurements. The surface O content decreases significantly from 45.62 to 30.38-39.85 at% from XPS measurements.
Supplementary Table 2. Comparison of HER and OER activity data among various catalysts.

| Catalysts  | Reactions | Tafel slope mV dec⁻¹ | η₀ mV | E_onset mV | j@200 mV mA cm⁻² | jₒ mA cm⁻² | TOF* s⁻¹ |
|------------|-----------|-----------------------|-------|------------|------------------|------------|----------|
| Fe-oxide   | HER       | 209                   | 505   | 94         | 0.6              | 0.0016     | 0.00374  |
|            | OER       | 207                   | 1.71  | 1.42       | -                | -          | 0.0141   |
| Pt/C       | HER       | 30                    | 13.7  | 0          | 610.0            | 0.7100     | 1.19000  |
| RuO₂       | OER       | 125                   | 1.40  | 1.29       | -                | -          | -        |
| IFONFs-15  | HER       | 96                    | 269   | 85         | 2.3              | 0.0012     | 0.00259  |
|            | OER       | 86                    | 1.61  | 1.44       | -                | -          | 0.0319   |
| IFONFs-30  | HER       | 68                    | 219   | 63         | 5.7              | 0.0470     | 0.00244  |
|            | OER       | 56                    | 1.52  | 1.43       | -                | -          | 0.1156   |
| IFONFs-45  | HER       | 31                    | 47    | 20         | 101.4            | 0.0950     | 0.27700  |
|            | OER       | 45                    | 1.49  | 1.39       | -                | -          | 0.2141   |
| IFONFs-60  | HER       | 55                    | 92    | 40         | 84.9             | 0.0322     | 0.09588  |
|            | OER       | 46                    | 1.51  | 1.40       | -                | -          | 0.1745   |
| IFONFs-90  | HER       | 63                    | 100   | 55         | 62.0             | 0.0260     | 0.07740  |
|            | OER       | 81                    | 1.61  | 1.42       | -                | -          | 0.0346   |
| Fe₂O₃      | HER       | 154                   | 456   | 124        | 0.4              | -          | -        |
|            | OER       | 120                   | 1.63  | 1.54       | -                | -          | -        |
| FeF₂       | HER       | 235                   | 610   | 147        | 0.3              | -          | -        |
|            | OER       | 182                   | 1.64  | 1.45       | -                | -          | -        |

* Note that the TOF for HER measured at η = 100 mV, for OER measured at η = 1.6 V, respectively.
Supplementary Table 3. Comparison of HER activity of Fe- and some non-Fe based catalysts.

| Catalysts                  | Electrolyte | Tafel slope (mV dec\(^{-1}\)) | Onset overpotential (mV) | \(\eta_{0}\) (mV) | Metal precursor | ref                       |
|----------------------------|-------------|--------------------------------|--------------------------|-------------------|-----------------|--------------------------|
| IFONFs-45                  | 1 M KOH     | 31                             | 20                       | 47                | Fe foil         | This work                |
| FeP nanorod arrays         | 1 M KOH     | 146                            | 86                       | 218               | Fe\(_2\)O\(_3\) nanorod arrays | ACS Catal., 2014\(^4\) |
| FeP                        | 1 M KOH     | 75                             | -                        | 194               | Fe\(_2\)O\(_3\) nanorod wires | Chem. Commun., 2016\(^5\) |
| FeP\(_2\)                  | 1 M KOH     | 67                             | -                        | 189               | Fe\(_2\)O\(_3\) nanorod wires | Chem. Commun., 2016\(^6\) |
| Porous Ni–Fe–P@C NRs       | 1 M KOH     | 92.6                           | –0                       | 79                | Iron(III) nitrate nonahydrate | J. Mater. Chem. A, 2017\(^7\) |
| Fe\(_0.1\)NiS\(_2\) NA/Ti | 1 M KOH     | 108                            | -                        | \(\eta_{0}=\) 243 | Fe(NO\(_3\))\(_3\)·6H\(_2\)O | Nano Res., 2016\(^8\) |
| NiFe-LDH NA/Ti             | 1 M KOH     | 124                            | -                        | \(\eta_{0}=\) 476 | Fe(NO\(_3\))\(_3\)·6H\(_2\)O | Nano Res., 2016\(^9\) |
| Ni\(_3\)Fe LDHs/NF         | 1 M KOH     | 75                             | -                        | 45                | Fe(NO\(_3\))\(_3\)·9H\(_2\)O | ACS Appl. Mater. Interfaces, 2016\(^10\) |
| NiFe/NF                    | 1 M KOH     | 112                            | -                        | 139               | FeSO\(_4\)·7H\(_2\)O | Int. J. Hydrogen Energ., 2016\(^11\) |
| Iron phosphide nanotubes   | 1 M KOH     | 59.5                           | 31                       | 120               | (Fe(NO\(_3\))\(_3\)·9H\(_2\)O | Chem.–Eur. J., 2015\(^12\) |
| (IPNTs)                    |             |                                |                          |                   |                 | Environ. Sci., 2016\(^13\) |
| EG/Co\(_{0.6}\)SeNiFe-LDH  | 1 M KOH     | 57                             | 240                      | 260               | Fe(NO\(_3\))\(_3\)·9H\(_2\)O | Adv. Mater., 2017\(^14\) |
| NiFe LDH-NS@DG10           | 1 M KOH     | 110                            | -                        | 300               | Fe(NO\(_3\))\(_3\)·9H\(_2\)O | Nat. Nano., 2017\(^15\) |
| Ru@C\(_2\)N\(_2\)          | 1 M KOH     | 38                             | -                        | 17                | RuCl\(_3\), NaBH\(_4\) | Nat.                     |
| 2.5H-PH NCMs\(_+\)        | 1 M KOH     | 38.1                           | -                        | 70                | (NH\(_4\))\(_2\)MoS\(_4\) | Nat.                     |
| HNDDDC\(_-\)               | 1 M KOH     | 93.4                           | -                        | 158               | Co(CH\(_3\))COO\(_2\)_ | Nat.                     |
| Catalyst                        | Support/Environment | % CO | T (°C) | Y (%) | Product | Reference |
|--------------------------------|---------------------|------|--------|-------|---------|-----------|
| 100,000-1,000/Co                |                     |      |        |       | CoO     | Commun., 2017 |
| 3.0 % S-CoO NRs                | 1 M KOH             | 82   | -      | 73    | CoO     | Commun., 2017 |
| RuCo@NC (S-4)                  | 1 M KOH             | 31   | -      | 28    | RuCl₃   | Commun., 2017 |

*Non-Fe based catalysts.*
Supplementary Table 4. Comparison of OER activity of Fe- and some non-Fe based catalysts.

| Catalysts                  | Electrolyte | Tafel slope mV dec\(^{-1}\) | Onset overpotential V | \(\eta_{10}\) V | Metal precursor | ref                                  |
|----------------------------|-------------|-------------------------------|-----------------------|----------------|----------------|--------------------------------------|
| IFONFs-45                  | 1 M KOH     | 45                            | 1.39                  | 1.49           | Fe foil        | ACS Appl. Mater. Interfaces, 2015\(^{18}\) |
| [Ni,Fe]O                   | 0.1 M KOH   | 36–48                         | -                     | 300 mV         | Metal chlorides| J. Mater. Chem. A, 2016\(^{19}\)      |
| FeP–rGO (70 : 30)@Au       | 1 M KOH     | 49.6                          | 1.44                  | 290 mV         | Triocetylphosphine oxide (TOPO) and Triocetylphosphine (TOP) | ACS Catal., 2014\(^{4}\) |
| Iron phosphide nanotubes (IPNTs) | 1 M KOH   | 43                            | 1.48                  | 1.52           | Fe(NO\(_3\)_3)·9H\(_2\)O | Chem.–Eur. J., 2015\(^{20}\) |
| FeP Na@CC                  | 1 M KOH     | 146                           | 86 mV                 | 218 mV         | Fe\(_2\)O\(_3\) nanorod arrays | Energ. Environ. Sci., 2015\(^{20}\) |
| Dc-LNiFeP/rGO              | 1 M KOH     | 33.6                          | 1.47                  | 1.50           | Fe(NO\(_3\)_3) | ACS Catal., 2012\(^{21}\) |
| Fe-Ni oxides               | 1 M KOH     | 51                            | -                     | -              | Iron nitrate   | J. Am. Chem. Soc., 2013\(^{22}\) |
| Ni-Fe LDH/CNT              | 1 M KOH     | 31                            | 1.45                  | 1.48           | Ferrous nitrate (Fe(NO\(_3\)_3) | Angew. Chem. Int. Ed., 2014\(^{23}\) |
| FeNi-rGO LDH               | 1 M KOH     | 39                            | 1.44                  | 1.436          | Ferrous chloride (FeCl\(_2\)) | Nano Res., 2014\(^{24}\) |
| NiFe LDHs                  | 1 M KOH     | 40                            | -                     | 300 mV         | Iron nitrate (Fe(NO\(_3\)_3)·9H\(_2\)O | Nat. Commun., 2014\(^{24}\) |
| Fe\(_2\)Ni\(_2\)O\(_4\)   | 1 M KOH     | 48                            | -                     | 286 mV         | Fe(NO\(_3\)_3) | Angew. Chem. Int. Ed., 2014\(^{25}\) |
| Porous Ni–Fe–P@C NRs       | 1 M KOH     | 40                            | 1.43                  | 217 mV         | Iron(III) nitrate nonahydrate | J. Mater. Chem. A, 2017\(^{25}\) |
| Fe\(_x\)Ni\(_2\)S\(_2\) Na/Ti | 1 M KOH   | 43                            | -                     | \(\eta_{10} \approx\) 231 mV | Fe(NO\(_3\)_3)·6H\(_2\)O | Nano Res., 2016\(^{2}\) |
| NSPM-Ni\(_x\)FeN/NF        | 1 M KOH     | 40                            | -                     | 1.495          | Iron nitrate Fe(NO\(_3\)_3)·9H\(_2\)O | ACS Appl. Mater. Interfaces, 2016\(^{3}\) |
| NiFe/NF                    | 1 M KOH     | 51                            | 1.58                  | 1.64           | FeSO\(_4\)·7H\(_2\)O | Int. J. Hydrogen Energ., 2016\(^{6}\) |
| NiFe-LDH NA/Ti             | 1 M KOH     | 117                           | -                     | \(\eta_{10} \approx\) 431 mV | Fe(NO\(_3\)_3)·6H\(_2\)O | Nano Res., 2016\(^{7}\) |
| Catalyst | KOH Molarity | OCP mV | Reference |
|----------|--------------|--------|-----------|
| EG/Co$_{0.85}$Se/NiFe-LDH | 1 M | 57 | 1.47 | 1.67 | Fe(NO$_3$)$_3$·9H$_2$O | *Energ. Environ. Sci.*, 2016$^{11}$ |
| NiFe LDH-NS@DG10 | 1 M | 52 | 1.41 | 210 mV | Fe(NO$_3$)$_3$·9H$_2$O | *Adv. Mater.*, 2017$^{12}$ |
| PrBa$_{0.5}$Sr$_{0.5}$Co$_{1.5}$Fe$_{0.5}$O$_{5+}$ (PBSCF-III) | 0.1 M | 52 | - | 358 mV | Fe(NO$_3$)$_3$·9H$_2$O | *Nat. Commun.*, 2017$^{26}$ |
| 2.5H-Ph | 1 M | 45.7 | - | 1.465 mV | (NH$_4$)$_2$MoS$_4$ | *Nat. Commun.*, 2017$^{18}$ |
| Ni-NHGF$^*$ | 1 M | 63 | 1.43 | 1.56 | NiCl$_2$·6H$_2$O | *Nat. Catal.*, 2018$^{27}$ |
| HNDDC-100,000-1,000/Co$^*$ | 1 M | 66.8 | - | 199 mV | Co(CH$_3$COO)$_2$ | *Nat. Commun.*, 2017$^{15}$ |

$^*$Non-Fe based catalysts.
## Supplementary Table 5. Comparison of HER and OER activity data among various catalysts.

| Catalysts | Reactions | Tafel slope mV dec⁻¹ | η₀ mV | η₁₀ mV | E_onset mV | ref |
|-----------|-----------|----------------------|-------|--------|-----------|-----|
| **Fluoride** | IFONFs-45 | HER | 31 | 47 | 199 | 20 | This work |
| Borides | FeB₂ | HER | 87.5 | 61 | 200ён | 20 | 28 |
| | Fe₂B | HER | 102.4 | 138 | 250ён | - | 28 |
| Sulfides | Fe₀.₁NiS₂ NA/Ti | HER | 108 | 250ён | 350ён | - | 7 |
| | (Ni₀.₇₅Fe₀.₂₅)Se₂ | HER | NA | NA | NA | NA | 29 |
| | FeP NAs/CC | HER | 146 | 218 | 275ён | 86 | 4 |
| | FeP NWs | HER | 75 | 194 | NA | - | 5 |
| | FeP₂ NWs | HER | 67 | 189 | NA | - | 10 |
| | Iron phosphide nanotube (IPNTs) | HER | 59.5 | 120 | 180ён | 31 | |
| | Nanoporous Fe₃N | HER | NA | NA | NA | NA | 30 |
| Nitrides/ Selenides | Co₃FeN₄ | HER | 94 | 23 | 147 | - | 31 |
| | Ni₃FeN-NPs | HER | 42 | 158 | 310ён | - | 32 |
| Carbides | Fe₃C@NG800-0.2 | HER | NA | NA | NA | NA | 33 |
| | IP-IC@SWNT(P) | HER | 87.6 | 301 | NA | - | 34 |
| | Fe@C-NG/NC NTs | OER | 163 | 1.68 | η₂₀ =1.72ён | - | 35 |

* The value is calculated from the curves shown in the literatures.
Supplementary Note 1: Synthesis of IFONFs.

Fe foils (0.05 mm, 99.5%, Advent Materials, UK) were used as substrates and cleaned and degreased by sonication in 2-propanol (~99.7%) and acetone (~99.9%) before use. Electrochemical anodic treatment was carried out at room temperature in a solution of 0.1 M NH₄F (98%, Alfa Aesar, USA) with 1 M deionized water in ethylene glycol (~99.9%) to grow Fe-oxide nanoporous layers on the Fe foils. Anodization was conducted at 40 V for 40 min in a two-electrode setup with platinum foil as a counter electrode. To grow thicker layers, extended growth duration is suggested. After that, the samples were immersed in ethanol overnight to remove the residual organic electrolyte in the nanoporous layer followed by fluorination. To convert the porous Fe-oxide to a porous iron fluoride-oxide film, the reaction with fluorine vapor was performed in a CVD apparatus. The Fe-oxide PTF was placed in the middle of a standard 1 in. quartz tube furnace and heated to 300-400 °C in Ar (100 sccm) at 6.4 Torr for different time (e.g. 15, 30, 45, 60, and 90 min), while ammonium fluoride (NH₄F, ~5 g) in a porcelain boat as a fluoride doping source was placed at the upstream side of the furnace far away from the center of heat region about 5 cm or heated by an external heating source at ~250 °C. The excess NH₄F was employed to ensure complete reaction between the Fe-oxide PTF and NH₄F. Ar (100 sccm) was used as a protective gas during the reaction and cooling process. At the same time, Fe₂O₃ PTF was prepared according our previous study by annealing at 350 °C for 3 h in air for comparison⁴⁶, and FeF₂ PTF was prepared through fluorination reaction with Fe₂O₃ PTF at 350 °C for 45 min.

Supplementary Note 2: Material characterization.

A JEOL 6500F SEM was used to investigate the morphology. A JEOL 2010 HRTEM was used to observe the morphologies and lattice fringes of the samples. The atomic resolution TEM and STEM structural characterizations of IFONFs were carried out with a probe-corrected Titan G2 60-300 (FEI, USA) and Titan ChemiSTEM (FEI, USA) at acceleration voltages of 300 kV and 200 kV, respectively. The crystal structure of the sample was evaluated using XRD analysis, which was performed by a Rigaku Dmax-2000 X-ray powder diffractometer with Cu Kα radiation (λ = 1.5418 Å). The operating voltage and current were kept at 40 kV and 40 mA, respectively. A semiquantitative estimation of the composition of the heterogeneous thin film was performed by MDI Jade 9 software. XPS was conducted on a PHI Quantera SXM scanning X-ray microscope. An Al anode at 25 W was used as an X-ray source with a pass-energy of 26.00 eV, 45 take off angle and a 100 μm beam size. A field-emission TEM (JEOL 2010F) with an imaging filter (Gatan GIF) was used at 200 kV to characterize the morphology and the particle size distribution of the synthesized products.

Supplementary Note 3: Electrode preparation and electrochemical characterization, HER and OER.

The IFONFs grown on Fe foil were directly used as working electrodes for the electrochemical measurements in a custom made two-compartment three-electrode electrochemical cell (Supplementary Fig. 25). Water electrolysis to generate H₂ and O₂ were performed at room temperature using a three-electrode configuration (CHI 660E) with IFONFs, a platinum wire, and a saturated calomel electrode (SCE) as working electrode, counter electrode, and reference
electrode, respectively. The polarization curves were obtained in 1 M KOH (pH = 14) alkaline solution with a scan rate of 50 mV s\(^{-1}\) at room temperature. The potential, measured against a SCE electrode, was converted to the potential versus the reversible hydrogen electrode (RHE) according to \(E_{\text{vs\,RHE}} = E_{\text{vs\,SCE}} + E^0_{\text{SCE}} + 0.059\,\text{pH}\). The presented current density was normalized to the geometric surface area. EIS were carried out at overpotential of -5 mV (vs RHE) with a frequency range of \(10^{-2}\) to \(10^6\) Hz with AC signal amplitude of 5 mV. Prior to all measurements, the electrochemical cell was purged with H\(_2\) bubbles for 30 min. The practical operations of the stability and durability were examined by electrolysis at fixed potentials in 1 M KOH over extended periods and long-term potential cycling.

**OER.** The polarization curves were obtained in O\(_2\)-saturated 1 M KOH (pH = 14) alkaline solution with a scan rate of 5 mV s\(^{-1}\) at room temperature. EIS measurements were performed by applying an AC voltage with 5 mV amplitude in a frequency range from \(10^{-2}\) to \(10^6\) Hz and recorded at 500 mV vs RHE. The stability test was performed by electrolysis at fixed potentials in 1 M KOH.

**Supplementary Note 4: Capacitance measurements and comparison of electrochemically active surface areas.**

The electrochemically active surface area (ECSA) was estimated from the electrochemical double-layer capacitance of the nanoporous layers. The \(C_{dl}\) was determined from the CV curves measured in a potential range without redox processes according to the following equation:

\[
C_{dl} = \frac{I_c}{\nu} \quad (1)
\]

where \(C_{dl}\), \(I_c\), and \(\nu\) are the double-layer capacitance (F cm\(^{-2}\)) of the electroactive materials, charging current (mA cm\(^{-2}\)), and scan rate (mV s\(^{-1}\)). The ECSA is then calculated from the double-layer capacitance according to equation:

\[
\text{ECSA} = \frac{C_{dl}}{C_s} \quad (2)
\]

Where, \(C_s\) is the capacitance of an atomically smooth planar surface of the material per unit area under identical electrolyte conditions. An average value of \(C_s = 40\,\mu\text{F cm}^{-2}\) is used in this work. The roughness factor (\(R_F\)) is then calculated by dividing the estimated ECSA by the geometric area of the electrode.

An alternative way is to calculate the double layer capacitance (\(C_{dl}\)) that is linearly proportional to effective active surface area and therefore can provide a relative comparison. The \(C_{dl}\) value can be estimated by plotting the \(J \,(J_a-J_c)\) at Supplementary Fig. 28a-b -0.075 V vs RHE, c-d 0.02 V vs RHE, e-f 0.01 V vs RHE, g-h 0.23 V vs RHE, i-j 0.01 V vs RHE, and k-l 0.22 V vs RHE against the scan rate, where the slope is double \(C_{dl}\). The linear relationships are observed with the slopes twice the \(C_{dl}\) value. Accordingly, the \(C_{dl}\) values for Fe-oxide, IFONFs-15, IFONFs-30 IFONFs-45 IFONFs-60, and IFONFs-90 are calculated to be 3.43, 13.13, 18.38, 63.40, 20.86, and 19.13 mF cm\(^{-2}\), respectively. Clearly, the IFONFs-45 shows the largest \(C_{dl}\), demonstrating its more catalytically active sites that profit from the defect enriched structure.

Calculated ECSA and \(R_F\) for the raw Fe-oxide PTF and IFONFs prepared with various time.

Fe-oxide PTF:
Fe$_2$O$_3$ oxide: \[ A_{\text{ECSA}}^{\text{Fe-oxide}} = \frac{3.43 \text{ mF cm}^{-2}}{40 \text{ µF cm}^{-2} \text{ per cm}^2 \text{ ECSA}} = 85.8 \text{ cm}^2 \text{ ECSA} \] (3)

\[ R_F^{\text{Fe-oxide}} = \frac{85.8 \text{ cm}^2 \text{ ECSA}}{1 \text{ cm}^2} = 85.8 \] (4)

IFONFs-15:

\[ A_{\text{ECSA}}^{\text{IFONFs-15}} = \frac{13.13 \text{ mF cm}^{-2}}{40 \text{ µF cm}^{-2} \text{ per cm}^2 \text{ ECSA}} = 328.3 \text{ cm}^2 \text{ ECSA} \] (5)

\[ R_F^{\text{IFONFs-15}} = \frac{328.3 \text{ cm}^2 \text{ ECSA}}{1 \text{ cm}^2} = 328.3 \] (6)

IFONFs-30:

\[ A_{\text{ECSA}}^{\text{IFONFs-30}} = \frac{18.38 \text{ mF cm}^{-2}}{40 \text{ µF cm}^{-2} \text{ per cm}^2 \text{ ECSA}} = 459.5 \text{ cm}^2 \text{ ECSA} \] (7)

\[ R_F^{\text{IFONFs-30}} = \frac{459.5 \text{ cm}^2 \text{ ECSA}}{1 \text{ cm}^2} = 459.5 \] (8)

IFONFs-45:

\[ A_{\text{ECSA}}^{\text{IFONFs-45}} = \frac{63.40 \text{ mF cm}^{-2}}{40 \text{ µF cm}^{-2} \text{ per cm}^2 \text{ ECSA}} = 1585.0 \text{ cm}^2 \text{ ECSA} \] (9)

\[ R_F^{\text{IFONFs-45}} = \frac{1585.0 \text{ cm}^2 \text{ ECSA}}{1 \text{ cm}^2} = 1585.0 \] (10)

IFONFs-60:

\[ A_{\text{ECSA}}^{\text{IFONFs-60}} = \frac{20.86 \text{ mF cm}^{-2}}{40 \text{ µF cm}^{-2} \text{ per cm}^2 \text{ ECSA}} = 521.5 \text{ cm}^2 \text{ ECSA} \] (11)

\[ R_F^{\text{IFONFs-60}} = \frac{521.5 \text{ cm}^2 \text{ ECSA}}{1 \text{ cm}^2} = 521.5 \] (12)

IFONFs-90:

\[ A_{\text{ECSA}}^{\text{IFONFs-90}} = \frac{19.13 \text{ mF cm}^{-2}}{40 \text{ µF cm}^{-2} \text{ per cm}^2 \text{ ECSA}} = 478.3 \text{ cm}^2 \text{ ECSA} \] (13)

\[ R_F^{\text{IFONFs-60}} = \frac{478.3 \text{ cm}^2 \text{ ECSA}}{1 \text{ cm}^2} = 478.3 \] (14)

In Supplementary Fig. 28, the $C_{dl}$ values for Fe$_2$O$_3$ PTF and FeF$_2$ PTF are calculated to be 16.28 and 13.38 mF cm$^{-2}$, respectively.

Calculated ECSA and $R_F$ for Fe$_2$O$_3$ PTF and FeF$_2$ PTF.

Fe$_2$O$_3$ PTF:

\[ A_{\text{ECSA}}^{\text{Fe2O3}} = \frac{16.28 \text{ mF cm}^{-2}}{40 \text{ µF cm}^{-2} \text{ per cm}^2 \text{ ECSA}} = 407 \text{ cm}^2 \text{ ECSA} \] (15)

\[ R_F^{\text{Fe2O3}} = \frac{407 \text{ cm}^2 \text{ ECSA}}{1 \text{ cm}^2} = 407 \] (16)
FeF$_2$ PTF:

\[ A_{\text{ECSA}}^{\text{FeF}_2} = \frac{13.38 \text{ mF cm}^{-2}}{40 \ \mu\text{F cm}^{-2 \text{ per cm}^2 \ ECSA}} = 334.5 \text{ cm}^2 \text{ECSA} \quad (17) \]

\[ R_{p}^{\text{FeF}_2} = \frac{334.5 \text{ cm}^2 \text{ECSA}}{1 \text{ cm}^2} = 334.5 \quad (18) \]

The exchange current density \( (j_0) \) was calculated using extrapolation methods. When the overpotential value is 0, the log \([j]\) values for IFONFs-45, IFONFs-30 and IFONFs-60 are -1.19, -0.78, and -0.63, respectively. Based on Tafel equations, \( j_0 \) for IFONFs-45, IFONFs-30 and IFONFs-60 was calculated to be 0.0950, 0.0470, and 0.0322 mA cm$^{-2}$, respectively.

**Supplementary Note 5: Calculation of TOF and the number of active sites for HER.**

For rough estimation of the active surface site density and per-site turn over frequency (TOF) in the IFONFs hybrid catalyst, we suppose that the contribution of the defect state plays a dominant role. This is reasonable since the catalytic performance of defect enriched IFONFs hybrid is far better than that of less defect catalyst. According to this approach adopted by Jaramillo et al$^{37}$, we carried out a similar calculation method by considering the relative roughness factor of the catalyst, the geometry of a IFONFs surface, and the hydrogen evolution current density. As shown in Fig. 4c of main text, we have determined the specific capacitance \( C_{\text{bulk}} \) of IFONFs-45 to be 63.40 mF cm$^{-2}$. And the \( C_{\text{bulk}} \) can be directly used to estimate the relevant electrochemical active surface area (ECSA) by using the specific capacitance value for a flat electrode with real surface area 1 cm$^2$.

We assume 40 \( \mu \text{F cm}^{-2} \) for a flat electrode for calculation the TOF values (Supplementary Table 2). Thus, the number of electrochemically effective surface sites on the IFONFs catalyst was calculated as the following:

\[ \frac{\text{# Surface sites (catalyst)}}{\text{cm}^2 \text{ geometric area}} = \frac{\text{# Surface sites (flat standard)}}{\text{cm}^2 \text{ geometric area}} \times \text{Roughness factor} \quad (19) \]

To further get insights into the per-site TOF, the following formula is utilized:

\[ \text{TOF per site} = \frac{\text{# Total Hydrogen Turn Overs} \text{ / cm}^2 \text{ geometric area}}{\text{# Surface sites (catalyst) / cm}^2 \text{ geometric area}} \quad (20) \]

The total number of hydrogen turn overs is related to the current density, and is calculated based on the following conversion:

\[ \# H_2 = \left( \frac{j \text{ mA}}{1000 \text{ mA}} \right) \left( \frac{1 \text{ Cs}^{-1}}{96485.3 \text{ C}} \right) \left( \frac{1 \text{ mol} H_2}{2 \text{ mol} e^{-1}} \right) \left( \frac{6.022 \times 10^{23} \text{ H}_2 \text{ molecules}}{2 \text{ mol} \ H_2} \right) = \]

\[ 3.12 \times 10^{25} \frac{H_2/5 \text{ cm}^2}{\text{mA cm}^2} \quad (21) \]

The upper limit of the number of active sites was calculated based on the hypothesis that all iron atoms in the IFONFs catalyst formed active Fe$_2$O$_7$-FeF$_2$ centers and all of them were accessible to the electrolyte. The real number of active and accessible iron sites should be considerably lower than the calculated value. The bulk iron content of IFONFs revealed by the ICP-MS measurement was about 19 wt%. The geometrical area of the electrode was 0.4 cm in diameter (~0.125 cm$^2$), and the mass of the electrode was found to be ~0.025 mg (measured based on the entire films) for each piece. So, the iron loading is equal to ~0.2 mg cm$^{-2}$. Accordingly, the upper limit of active site density is
\[
\frac{19 \text{ mg}}{100 \text{ mg}} \times 0.2 \text{ mg/cm}^2 \times \frac{1 \text{ mmol}}{55.85 \text{ mg}} \times 6.022 \times 10^{20} \text{ sites/mmol} = 0.410 \times 10^{18} \text{ sites cm}^{-2} \quad (22)
\]

Accordingly, at an overpotential of 100 mV, the HER current density for Fe-oxide, IFONFs-15, IFONFs-30, IFONFs-45, IFONFs-60, and IFONFs-90 were 0.370, 0.340, 0.320, 36.4, 12.6, and 10.16 mA cm\(^{-2}\), respectively, and the TOF value of Fe-oxide was calculated to be

\[
\text{TOF}_{\text{Fe-oxide}} = \frac{3.12 \times 10^{15} \text{ XH}_2/\text{cm}^2 \text{ per mA/cm}^2 \times 0.492 \text{ mA/cm}^2}{0.410 \times 10^{18} \text{ sites/cm}^2} = 0.00374 \text{ s}^{-1} \quad (23)
\]

\[
\text{TOF}_{\text{IFONFs–15}} = \frac{3.12 \times 10^{15} \text{ XH}_2/\text{cm}^2 \text{ per mA/cm}^2 \times 0.34 \text{ mA/cm}^2}{0.410 \times 10^{18} \text{ sites/cm}^2} = 0.00259 \text{ s}^{-1} \quad (24)
\]

\[
\text{TOF}_{\text{IFONFs–30}} = \frac{3.12 \times 10^{15} \text{ XH}_2/\text{cm}^2 \text{ per mA/cm}^2 \times 0.32 \text{ mA/cm}^2}{0.410 \times 10^{18} \text{ sites/cm}^2} = 0.00244 \text{ s}^{-1} \quad (25)
\]

\[
\text{TOF}_{\text{IFONFs–45}} = \frac{3.12 \times 10^{15} \text{ XH}_2/\text{cm}^2 \text{ per mA/cm}^2 \times 36.4 \text{ mA/cm}^2}{0.410 \times 10^{18} \text{ sites/cm}^2} = 0.27700 \text{ s}^{-1} \quad (26)
\]

\[
\text{TOF}_{\text{IFONFs–60}} = \frac{3.12 \times 10^{15} \text{ XH}_2/\text{cm}^2 \text{ per mA/cm}^2 \times 12.6 \text{ mA/cm}^2}{0.410 \times 10^{18} \text{ sites/cm}^2} = 0.09588 \text{ s}^{-1} \quad (27)
\]

\[
\text{TOF}_{\text{IFONFs–90}} = \frac{3.12 \times 10^{15} \text{ XH}_2/\text{cm}^2 \text{ per mA/cm}^2 \times 10.3 \text{ mA/cm}^2}{0.410 \times 10^{18} \text{ sites/cm}^2} = 0.07762 \text{ s}^{-1} \quad (28)
\]

Since the difficulty in attributing the observed peaks to a given redox couple, the number of active sites should be proportional to the integrated charge over the CV curve (Supplementary Fig. 30). Assuming a one-electron process for both reduction and oxidation, the upper limit of active sites \(n\) for IFONFs-45 could be calculated according to the follow equation:

\[
n = \frac{Q}{2F} \quad (29)
\]

where \(F\) and \(Q\) are the Faraday constant and the whole charge of CV curve, respectively.

\[
n_{\text{pt/C}} = \frac{0.2776}{2 \times 96485} = 1.44 \times 10^{-6} \quad (30)
\]

\[
n_{\text{IFONFs–30}} = \frac{0.0374}{2 \times 96485} = 1.94 \times 10^{-7} \quad (31)
\]

\[
n_{\text{IFONFs–45}} = \frac{0.2096}{2 \times 96485} = 1.09 \times 10^{-6} \quad (32)
\]

\[
n_{\text{IFONFs–60}} = \frac{0.0436}{2 \times 96485} = 2.26 \times 10^{-7} \quad (33)
\]

Supplementary Note 6: Calculation of TOF the number of active sites for OER.

The values of TOF for OER were calculated by assuming that every metal atom was involved in the catalysis (lower limits):

\[
\text{TOF} = \frac{J}{4xFxn} \quad (34)
\]

where \(J\) is the current density (A cm\(^{-2}\)), \(F\) is Faraday’s constant (96485.3 C mol\(^{-1}\)) and \(n\) is moles of electrocatalysts (mol cm\(^{-2}\)). Accordingly, at an overpotential of 1.6 V, the OER current density for Fe-oxide, IFONFs-15, IFONFs-30, IFONFs-45, IFONFs-60, and IFONFs-90 were 3.7, 8.4, 30.4, 56.3, 45.9, and 9.1 mA cm\(^{-2}\), respectively, and the corresponding TOF values were calculated to be
The generated gas was confirmed by gas chromatography (GC) analysis and measured quantitatively using a calibrated pressure sensor to monitor the pressure change in the cathode compartment of an H-type electrolytic cell. The Faradic efficiency was calculated by comparing the amount of measured hydrogen generated by galvanostatic electrolysis with calculated hydrogen (assuming 100% FE). The rough agreement of both values (Supplementary Fig. 41) suggests nearly 100% FE for HER and OER in 1 M KOH. GC analysis was carried out on GC–2014C (Shimadzu Co.) with thermal conductivity detector and nitrogen carrier gas. Pressure data during electrolysis were recorded using a CEM DT-8890 Differential Air Pressure Gauge.

TOF$_{\text{Fe-oxide}}$ = \frac{3.7 \times mA \text{cm}^{-2}}{4 \times 96485.3 \text{ C mol}^{-1}} \times \frac{19 \text{ mg}}{100 \text{ mg}} \times \frac{1 \text{ mmol}}{55.85 \text{ mg}} = 0.0141 \text{ s}^{-1} \quad (35)

TOF$_{\text{IFONFs-15}}$ = \frac{8.4 \times mA \text{cm}^{-2}}{4 \times 96485.3 \text{ C mol}^{-1}} \times \frac{19 \text{ mg}}{100 \text{ mg}} \times \frac{1 \text{ mmol}}{55.85 \text{ mg}} = 0.0319 \text{ s}^{-1} \quad (36)

TOF$_{\text{IFONFs-30}}$ = \frac{30.4 \times mA \text{cm}^{-2}}{4 \times 96485.3 \text{ C mol}^{-1}} \times \frac{19 \text{ mg}}{100 \text{ mg}} \times \frac{1 \text{ mmol}}{55.85 \text{ mg}} = 0.1156 \text{ s}^{-1} \quad (37)

TOF$_{\text{IFONFs-45}}$ = \frac{56.3 \times mA \text{cm}^{-2}}{4 \times 96485.3 \text{ C mol}^{-1}} \times \frac{19 \text{ mg}}{100 \text{ mg}} \times \frac{1 \text{ mmol}}{55.85 \text{ mg}} = 0.2141 \text{ s}^{-1} \quad (38)

TOF$_{\text{IFONFs-60}}$ = \frac{45.9 \times mA \text{cm}^{-2}}{4 \times 96485.3 \text{ C mol}^{-1}} \times \frac{19 \text{ mg}}{100 \text{ mg}} \times \frac{1 \text{ mmol}}{55.85 \text{ mg}} = 0.1745 \text{ s}^{-1} \quad (39)

TOF$_{\text{IFONFs-90}}$ = \frac{9.1 \times mA \text{cm}^{-2}}{4 \times 96485.3 \text{ C mol}^{-1}} \times \frac{19 \text{ mg}}{100 \text{ mg}} \times \frac{1 \text{ mmol}}{55.85 \text{ mg}} = 0.0346 \text{ s}^{-1} \quad (40)

A linear plot between the oxidation currents for redox species and scan rates can be derived from cyclic voltammograms, and the corresponding slopes can be obtained from the linear plots (Supplementary Fig. 36). The quantity of active species (m) is calculated based on the formula: slope = nF2m/4RT, where n is the number of electrons transferred, which is denoted as 1 in order to achieve the upper limit in the concentration of active sites, F is the Faradic constant (96485 C mol$^{-1}$), m is the number of active species, and R and T are the ideal gas constant (8.314 J mol$^{-1}$K$^{-1}$) and absolute temperature (298 K), respectively. The results showed that the number of active sites for IFONFs-45 is 2.59×10$^{-8}$ mol, much larger than that of IFONFs-30 (1.26×10$^{-8}$ mol) and IFONFs-60 (1.50×10$^{-8}$ mol).

\[ m_{\text{Fe-oxide}} = \frac{0.00406+4.314+298}{96485+96485} = 4.31 \times 10^{-9} \text{ mol} \quad (41) \]

\[ m_{\text{IFONFs-15}} = \frac{0.00646+4.314+298}{96485+96485} = 6.88 \times 10^{-9} \text{ mol} \quad (42) \]

\[ m_{\text{IFONFs-30}} = \frac{0.01181+4.314+298}{96485+96485} = 1.26 \times 10^{-8} \text{ mol} \quad (43) \]

\[ m_{\text{IFONFs-45}} = \frac{0.02431+4.314+298}{96485+96485} = 2.59 \times 10^{-8} \text{ mol} \quad (44) \]

\[ m_{\text{IFONFs-60}} = \frac{0.0141+4.314+298}{96485+96485} = 1.50 \times 10^{-8} \text{ mol} \quad (45) \]

\[ m_{\text{IFONFs-90}} = \frac{0.00791+4.314+298}{96485+96485} = 8.42 \times 10^{-9} \text{ mol} \quad (46) \]

**Supplementary Note 7: Determination of Faradaic efficiency**

The generated gas was confirmed by gas chromatography (GC) analysis and measured quantitatively using a calibrated pressure sensor to monitor the pressure change in the cathode compartment of an H-type electrolytic cell. The Faradic efficiency was calculated by comparing the amount of measured hydrogen generated by galvanostatic electrolysis with calculated hydrogen (assuming 100% FE). The rough agreement of both values (Supplementary Fig. 41) suggests nearly 100% FE for HER and OER in 1 M KOH. GC analysis was carried out on GC–2014C (Shimadzu Co.) with thermal conductivity detector and nitrogen carrier gas. Pressure data during electrolysis were recorded using a CEM DT-8890 Differential Air Pressure Gauge.
Supplementary Note 8: Computational methods.

We performed spin-polarized Density Functional Theory (DFT) calculations with the LDA+U approach by using Vienna Ab-initio Simulation Package (VASP)\textsuperscript{38}. Specifically, the projector augmented wave (PAW) method for potentials at the core region\textsuperscript{39,40} and the generalized gradient approximation (GGA) of Perdew–Burke–Ernzerhof (PBE) exchange-correlation functional were adopted\textsuperscript{41,42,43}. A $U = 5$ eV was used to correct the correlation of Fe d-electrons\textsuperscript{44}. A kinetic energy cut-off of 400 eV was used for the plane-wave expansion, and all atomic positions were fully relaxed with a $\Gamma$ point until the final force on each atom was less than 0.01 eV/Å.

Atomic coordinates of FeF$_2$ (110) surface, with stoichiometric termination, and with O-Fe dimer adsorption. The corresponding configurations with H adsorption are also provided. The coordinates are listed in VASP CONTCAR format.

per woH

\begin{verbatim}
 1.00000000000000  13.367000000000009  0.0000000000000000  0.0000000000000000
  0.0000000000000000  13.5719200000000004  0.0000000000000000
  0.0000000000000000  0.0000000000000000   25.0000000000000000

Fe   F

64   128
\end{verbatim}

Selective dynamics

Direct

\begin{verbatim}
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0.1965432843015685  0.2497170521389195  0.7467951620810844  T   T   T
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| 0.6934712016717242 | 0.9998274801287134 | 0.6028116304872940 | T | T | T |
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| 0.9416805528497363 | 0.4999665157021388 | 0.3286952833876105 | T | T | T |
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| 0.0711234273903660 | 0.9998783935563189 | 0.7380768645366991 | T | T | T |
| 0.3169502972052269 | 0.2497417948274141 | 0.3374827329829518 | T | T | T |
| 0.3177728854238150 | 0.4997688623913119 | 0.4680487390088382 | T | T | T |
| 0.3179500168985119 | 0.2496818654757503 | 0.6071470000671167 | T | T | T |
|---------------------|---------------------|---------------------|---|---|---|
| 0.3211243683388344  | 0.9997951627730368  | 0.7380889857116422 | T | T | T |
| 0.0669472802049558  | 0.7500228170271869  | 0.3375411888844361 | T | T | T |
| 0.0677542995227141  | 0.9997586569469072  | 0.4680531269281242 | T | T | T |
| 0.0678991681286884  | 0.7496701430220248  | 0.6071401513716870 | T | T | T |
| 0.0711332805573857  | 0.4998781751349582  | 0.7380806631951254 | T | T | T |
| 0.3170039908596254  | 0.7497972962088467  | 0.3375228355989918 | T | T | T |
| 0.3177744310547566  | 0.9997616540226778  | 0.4680241664074176 | T | T | T |
| 0.3179815261380611  | 0.7496746009212180  | 0.6071340336613222 | T | T | T |
| 0.3211338443160160  | 0.4998111358036295  | 0.7380955260747399 | T | T | T |
| 0.5669198527677058  | 0.2499804117382181  | 0.3375440136389701 | T | T | T |
| 0.5677839334782265  | 0.4997653082501614  | 0.4680493815348043 | T | T | T |
| 0.5679003737379558  | 0.2496738115529065  | 0.6071742859400869 | T | T | T |
| 0.5711291903062230  | 0.9998915617235429  | 0.7380996643545273 | T | T | T |
| 0.8169773361867843  | 0.2499764001267319  | 0.3375881941193852 | T | T | T |
| 0.8178009688710469  | 0.4997863803651175  | 0.4680446239697580 | T | T | T |
| 0.8179813382477097  | 0.2496808737885215  | 0.6071601428694299 | T | T | T |
| 0.8211200600912598  | 0.9997825063792565  | 0.7381112784017800 | T | T | T |
| 0.5669780909694900  | 0.7499683268585492  | 0.3375340921836553 | T | T | T |
| 0.5677686418931335  | 0.9998050892812512  | 0.4680469997667638 | T | T | T |
| 0.5679023726524500  | 0.7496828826757752  | 0.6071558342465748 | T | T | T |
| 0.5711437225824280  | 0.4998843473741462  | 0.7380909326391243 | T | T | T |
| 0.8169845225964122  | 0.7499330242409890  | 0.3375272606505391 | T | T | T |
| 0.8177319250488406  | 0.9998004683419959  | 0.4680765393748467 | T | T | T |
| 0.8179489865309852  | 0.7496802986549264  | 0.6071410776027480 | T | T | T |
| 0.8211284443997124  | 0.4997982783048419  | 0.7380994678510432 | T | T | T |
| 0.0676277583293859  | 0.9993546203107568  | 0.3872545976183356 | T | T | T |
|       |       |       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| 0.0677612833816070 | 0.2499206822515370 | 0.5259337100300673 | T | T | T | T | T | T | T | T | T |
| 0.068694786962736 | 0.0005967376726773 | 0.6566723897930223 | T | T | T | T | T | T | T | T | T |
| 0.1914677958753090 | 0.3410003233460753 | 0.3290872984131647 | T | T | T | T | T | T | T | T | T |
| 0.1927754375610591 | 0.0999935299071189 | 0.4693140308645663 | T | T | T | T | T | T | T | T | T |
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| 0.0663140554427427 | 0.0001630705008053 | 0.2846209807133346 | T | T | T | T | T | T | T | T | T |
| 0.067458970399953 | 0.2500445798771526 | 0.4188708152583013 | T | T | T | T | T | T | T | T | T |
| 0.0682373454760996 | 0.496938527577232 | 0.5493484333224253 | T | T | T | T | T | T | T | T | T |
| 0.067193090437884 | 0.2485293014396303 | 0.6879490002697231 | T | T | T | T | T | T | T | T | T |
| 0.1924768678492033 | 0.1586188672442415 | 0.3295260082753690 | T | T | T | T | T | T | T | T | T |
| 0.1927680901355508 | 0.3996985508567003 | 0.4697561694843372 | T | T | T | T | T | T | T | T | T |
| 0.1929728040209146 | 0.149618646104357 | 0.6050252828197187 | T | T | T | T | T | T | T | T | T |
| 0.193756054229532 | 0.4083513650493423 | 0.7455087516528395 | T | T | T | T | T | T | T | T | T |
| 0.0729254264000086 | 0.2507322642752313 | 0.7908081163654882 | T | T | T | T | T | T | T | T | T |
| 0.3177804061124329 | 0.9993291520444274 | 0.3872142248016874 | T | T | T | T | T | T | T | T | T |
| 0.3177308862655148 | 0.2499026826865233 | 0.5259216234549347 | T | T | T | T | T | T | T | T | T |
| 0.3187499008570380 | 0.0005695380340841 | 0.6566855598191845 | T | T | T | T | T | T | T | T | T |
| 0.4414840750792287 | 0.3409705248653396 | 0.3290506879222617 | T | T | T | T | T | T | T | T | T |
| 0.4427193353851859 | 0.0997778319354414 | 0.4693496701926529 | T | T | T | T | T | T | T | T | T |
| 0.4429682199203659 | 0.3499856442395971 | 0.6057328350212997 | T | T | T | T | T | T | T | T | T |
| 0.4483135717139418 | 0.0908519001374144 | 0.7474896348039497 | T | T | T | T | T | T | T | T | T |
| 0.3164400487716008 | 1.0000335975404400 | 0.2845357967376157 | T | T | T | T | T | T | T | T | T |
| 0.3175569881232617 | 0.2502230401595517 | 0.4188244381281387 | T | T | T | T | T | T | T | T | T |
| 0.3182480861464659 | 0.4996468537764230 | 0.5493604698954725 | T | T | T | T | T | T | T | T | T |
| 0.3173210537713232 | 0.2486542889614005 | 0.6879704674539062 | T | T | T | T | T | T | T | T | T |
| 0.4424094385179723 | 0.1585802024687236 | 0.3295619430401234 | T | T | T | T | T | T | T | T | T |
| x       | y       | width  | height | region               | label | features |
|---------|---------|--------|--------|----------------------|-------|----------|
| 0.4427281561396595 | 0.3996740116619801 | 0.4699694116349039 | T | T | T |
| 0.4429443758032360 | 0.1496311375539466 | 0.6050122754084738 | T | T | T |
| 0.4437933938452192 | 0.4083697590996802 | 0.7455186223306765 | T | T | T |
| 0.3228908659223078 | 0.2508709838310484 | 0.7908682781556431 | T | T | T |
| 0.0679516574568566 | 0.4993713648080856 | 0.3872380199271537 | T | T | T |
| 0.0677273279669021 | 0.7499132931374247 | 0.5259214172375215 | T | T | T |
| 0.0686627026639820 | 0.5006713713781823 | 0.6566765670641073 | T | T | T |
| 0.1916385246356772 | 0.8410140830563483 | 0.3291864735198887 | T | T | T |
| 0.1927937382678032 | 0.6000176860494872 | 0.4693653539044920 | T | T | T |
| 0.1929779649998231 | 0.8499770105798868 | 0.6055549429784115 | T | T | T |
| 0.1984439738497653 | 0.5908381859222038 | 0.7474836467759701 | T | T | T |
| 0.066155462075956 | 0.5002278672385710 | 0.2845781362167785 | T | T | T |
| 0.0675170324331336 | 0.7502227178818200 | 0.4188737217875176 | T | T | T |
| 0.0682540933348270 | 0.9996171985163791 | 0.5493497192796827 | T | T | T |
| 0.0672116431629692 | 0.7485240531159567 | 0.6879370821315538 | T | T | T |
| 0.1923394753513061 | 0.6586918295694991 | 0.3295530685676358 | T | T | T |
| 0.1927925810125524 | 0.8996998055890075 | 0.4697678978732557 | T | T | T |
| 0.1929845067769082 | 0.6496371196515446 | 0.6049972214931277 | T | T | T |
| 0.1938154841086185 | 0.9083488250281380 | 0.745520563774981 | T | T | T |
| 0.0730393921194966 | 0.7507223036297918 | 0.7907958161555388 | T | T | T |
| 0.3179212200568615 | 0.4993908536080167 | 0.3872444423333184 | T | T | T |
| 0.3178037269017414 | 0.7499005963993821 | 0.5259180370330861 | T | T | T |
| 0.3187574594047151 | 0.5006487309366148 | 0.6566940783033506 | T | T | T |
| 0.4416297271960118 | 0.8410311681953072 | 0.3291771334844147 | T | T | T |
| 0.4427745041720852 | 0.500000547645884130 | 0.4694139429505366 | T | T | T |
| 0.4429896402944282 | 0.8500033560893254 | 0.60566164717537222 | T | T | T |
| 0.4484256745579187 | 0.5908530612793446 | 0.7475397778211329 | T | T | T |
| Value 1 | Value 2 | Value 3 | Result 1 | Result 2 | Result 3 | Result 4 | Result 5 | Result 6 |
|--------|--------|--------|----------|----------|----------|----------|----------|----------|
| 0.3162778351520767 | 0.5004110093440020 | 0.2845903985664170 | T | T | T | T | T | T |
| 0.3176219262636087 | 0.7500163719760098 | 0.4188619945646858 | T | T | T | T | T | T |
| 0.3182686046545439 | 0.9997187316150321 | 0.5493402675711343 | T | T | T | T | T | T |
| 0.3173236625925244 | 0.7486349570500910 | 0.6879510673978133 | T | T | T | T | T | T |
| 0.4424421181675193 | 0.6586518886428802 | 0.3295158851206005 | T | T | T | T | T | T |
| 0.4427905713003590 | 0.8996862039590011 | 0.4699653015068563 | T | T | T | T | T | T |
| 0.4429817162557794 | 0.6496122328220370 | 0.6049552603821452 | T | T | T | T | T | T |
| 0.4438858312429836 | 0.9083857193887468 | 0.7455379142322571 | T | T | T | T | T | T |
| 0.3229934692258419 | 0.7508818688519874 | 0.7908662561983916 | T | T | T | T | T | T |
| 0.5678340426863137 | 0.9993969591012232 | 0.387228584483481 | T | T | T | T | T | T |
| 0.5676708864137142 | 0.2499109244131953 | 0.5259473846942025 | T | T | T | T | T | T |
| 0.5686722404483620 | 0.0005575267698437 | 0.6566932105352457 | T | T | T | T | T | T |
| 0.6916215093971931 | 0.3411469918481433 | 0.3292806184019646 | T | T | T | T | T | T |
| 0.6927335855630905 | 0.1000318916738155 | 0.4693978716455005 | T | T | T | T | T | T |
| 0.6929773862497667 | 0.3499895522670254 | 0.6055930467058535 | T | T | T | T | T | T |
| 0.6983205269870022 | 0.0908290653485181 | 0.7475449343239804 | T | T | T | T | T | T |
| 0.5663216620842989 | 0.0002307661447936 | 0.2845722328060017 | T | T | T | T | T | T |
| 0.5674648162714661 | 0.2500929162857772 | 0.4188807580845390 | T | T | T | T | T | T |
| 0.5682384147594295 | 0.4996056548617134 | 0.5493504853209609 | T | T | T | T | T | T |
| 0.5673345551925207 | 0.2485442402066211 | 0.6879722659242048 | T | T | T | T | T | T |
| 0.6923214725581994 | 0.1588171050346226 | 0.3295323599288967 | T | T | T | T | T | T |
| 0.6927974691810370 | 0.3997100940903646 | 0.4697735226260951 | T | T | T | T | T | T |
| 0.6929719077317749 | 0.1496430925577186 | 0.6050449300437405 | T | T | T | T | T | T |
| 0.6937497559638561 | 0.4083619487711203 | 0.7455271435874348 | T | T | T | T | T | T |
| 0.5728852151282473 | 0.2507998898534207 | 0.7908139116383780 | T | T | T | T | T | T |
| 0.8178232190340858 | 0.9995364005010333 | 0.387282492838882 | T | T | T | T | T | T |
| 0.8177459723870398 | 0.2499430416565546 | 0.5259508199600507 | T | T | T | T | T | T |
| Value   | Value   | Value   | Value   | Value   | Value   | Value   | Value   | Value   | Value   |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|
| 0.818755259692515 | 0.0006738081565186 | 0.6567073148851740 | T | T | T |
| 0.9414401115019583 | 0.3411999136299322 | 0.3292003730473957 | T | T | T |
| 0.9427588354295587 | 0.0999594865500355 | 0.4694700985507810 | T | T | T |
| 0.9429992143169221 | 0.3500103696899060 | 0.6056775357116951 | T | T | T |
| 0.9483022797113331 | 0.0908077923528833 | 0.7475449789222469 | T | T | T |
| 0.8164083051028693 | 0.0005518696995715 | 0.2846253577390207 | T | T | T |
| 0.8175871084243399 | 0.2500162112981177 | 0.4189204140964652 | T | T | T |
| 0.8182456479951365 | 0.4996948324872780 | 0.549357203773914 | T | T | T |
| 0.8174208927396669 | 0.2486084168885133 | 0.6879765388866346 | T | T | T |
| 0.9425152458675271 | 0.1588050792756338 | 0.3295612611287150 | T | T | T |
| 0.9427675007894131 | 0.3996860017588950 | 0.469977246644718 | T | T | T |
| 0.9429729571903857 | 0.1496172891827927 | 0.6049463611189531 | T | T | T |
| 0.9438191882821914 | 0.4083596471689280 | 0.7455293228521198 | T | T | T |
| 0.8228857213717569 | 0.2508930261923951 | 0.7908696607306221 | T | T | T |
| 0.5677712480382390 | 0.4993384439108956 | 0.3872330982124340 | T | T | T |
| 0.5677410693620932 | 0.7499656300513114 | 0.5259367152113531 | T | T | T |
| 0.5686855029678246 | 0.5005971168709021 | 0.6566841736112401 | T | T | T |
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| 0.6928045754896406 | 0.5999899152442558 | 0.4693614870365656 | T | T | T |
| 0.6929607685192800 | 0.850065747341522 | 0.6055927455137292 | T | T | T |
| 0.6984395597374060 | 0.5908524009214955 | 0.7475054593882464 | T | T | T |
| 0.5661911116515459 | 0.5000460776958231 | 0.2845932047017235 | T | T | T |
| 0.5675274671424815 | 0.7501014152674390 | 0.418869457083697 | T | T | T |
| 0.5682360627673473 | 0.9997412604497878 | 0.5493547445926469 | T | T | T |
| 0.5671972468881219 | 0.7485409868754213 | 0.6879569330094736 | T | T | T |
| 0.6923707278735455 | 0.6587453199871390 | 0.3295060890284872 | T | T | T |
| 0.6927156037526481 | 0.8997107539910408 | 0.4697527116682546 | T | T | T |
| x    | y    | z    | T  | T  | T |
|------|------|------|----|----|----|
| 0.692572941202671 | 0.6496275471615750 | 0.6050238607601280 | T  | T  | T |
| 0.6938405879025332 | 0.9083663528136687 | 0.7455301963216506 | T  | T  | T |
| 0.5730429258221638 | 0.7507958962944057 | 0.7908144536162698 | T  | T  | T |
| 0.8179858992497830 | 0.4994706364281405 | 0.3872315079518212 | T  | T  | T |
| 0.8177285928829264 | 0.7498362940696583 | 0.5259210801997456 | T  | T  | T |
| 0.8187567408619942 | 0.5006150615231991 | 0.6566949365633457 | T  | T  | T |
| 0.9414960266418378 | 0.8411577542738149 | 0.3291544534111324 | T  | T  | T |
| 0.9427869283877661 | 0.5999867868202573 | 0.4693647820180850 | T  | T  | T |
| 0.9429637467462408 | 0.8499947586031656 | 0.6056835621879487 | T  | T  | T |
| 0.9483942154426700 | 0.5908409281871149 | 0.7475217669942207 | T  | T  | T |
| 0.8162843554313153 | 0.5005254491305974 | 0.2845641168712997 | T  | T  | T |
| 0.8175607812744962 | 0.7500858225072773 | 0.418862041670704  | T  | T  | T |
| 0.8182268361605285 | 0.9996856405017883 | 0.5493847716917167 | T  | T  | T |
| 0.8172891366288426 | 0.7486548173210940 | 0.6879571284884933 | T  | T  | T |
| 0.9424701010685564 | 0.6587666669760283 | 0.329541035304434  | T  | T  | T |
| 0.9426642097926021 | 0.8996844340850672 | 0.4700006546771913 | T  | T  | T |
| 0.9429371042565502 | 0.6496389285183793 | 0.6049548640088731 | T  | T  | T |
| 0.9439130487730724 | 0.9083506260138228 | 0.7454912773418328 | T  | T  | T |
| 0.8230251582724574 | 0.7508928967659457 | 0.7908652121336062 | T  | T  | T |

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Selective dynamics
|               | Direct          |               |               |               |
|---------------|----------------|---------------|---------------|---------------|
| 0.1917951254792667 | 0.9998249521814799 | 0.3283341279839310 | T | T | T |
| 0.1926745915647252  | 0.2498831746710497  | 0.4725900044550574 | T | T | T |
| 0.1943300150641639  | 0.4998372710750746  | 0.6036434999311172  | T | T | T |
| 0.1965497903515102  | 0.2496829406366773  | 0.7469720808756088  | T | T | T |
| 0.4417822411761595  | 0.9998360562700570  | 0.3284074993741303  | T | T | T |
| 0.4426350285156927  | 0.2498604908420114  | 0.472639214462588  | T | T | T |
| 0.4426490117790164  | 0.4998044935244382  | 0.6036629019934611  | T | T | T |
| 0.4463358739827160  | 0.2496402564949123  | 0.7470102702854554  | T | T | T |
| 0.1917025868995014  | 0.4998692627246545  | 0.3283436799310159  | T | T | T |
| 0.1926931029379870  | 0.7498358908534599  | 0.4726032947752831  | T | T | T |
| 0.1934971193971030  | 0.9997961259108543  | 0.6027042367449558  | T | T | T |
| 0.1966325734342110  | 0.7498542734783656  | 0.7469353284923585  | T | T | T |
| 0.4417318046495201  | 0.4998467024017007  | 0.3284370842399023  | T | T | T |
| 0.4426857028965414  | 0.7497782838864302  | 0.4726502681038466  | T | T | T |
| 0.4434195981737010  | 0.9998097679837293  | 0.6027120414339844  | T | T | T |
| 0.4464232635847649  | 0.7498552251549742  | 0.7470213962359279  | T | T | T |
| 0.6918047673325677  | 0.9999550883000163  | 0.3283608677965357  | T | T | T |
| 0.6926413172260879  | 0.2498993893541530  | 0.4726216104764108  | T | T | T |
| 0.6933842646911484  | 0.9998014971804983  | 0.6026323027341425  | T | T | T |
| 0.6965026967906975  | 0.2497253998611320  | 0.7469847547762227  | T | T | T |
| 0.9417799710482637  | 0.9999556591764215  | 0.3284758181011318  | T | T | T |
| 0.9426771286025224  | 0.2498409253283063  | 0.4726684706423913  | T | T | T |
| 0.9435066535418620  | 0.4998235984658696  | 0.6026256778732777  | T | T | T |
| 0.9463836298264715  | 0.2496988964941619  | 0.747001755306130  | T | T | T |
| 0.691720877438683  | 0.9999236859459329  | 0.3283535291994759  | T | T | T |
| 0.6926694178558396  | 0.7498350058017276  | 0.4725984084431707  | T | T | T |
| Value 1 | Value 2 | Value 3 | Value 4 | Value 5 | Value 6 | Value 7 | Value 8 | Value 9 | Value 10 | Value 11 | Value 12 |
|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| 0.6934645250088228 | 0.9998092965148061 | 0.6027384735437630 | T | T | T |
| 0.6965732424531494 | 0.7497547875696244 | 0.7469634868916405 | T | T | T |
| 0.9417309023923851 | 0.4999626410195396 | 0.3284375398692541 | T | T | T |
| 0.9426704178522901 | 0.7498191319140144 | 0.4726346817849594 | T | T | T |
| 0.9434174756583652 | 0.9998047665890007 | 0.6027212997956374 | T | T | T |
| 0.9464763451518605 | 0.7497384636817713 | 0.7469884356423556 | T | T | T |
| 0.0669379852262806 | 0.2500022112406367 | 0.3375343159708528 | T | T | T |
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| X         | Y         | Z         | W         | X         | Y         | Z         | W         | X         | Y         | Z         | W         |
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| Value 1 | Value 2 | Value 3 | Value 4 | Value 5 | Value 6 | Value 7 | Value 8 | Value 9 | Value 10 | Value 11 | Value 12 | Value 13 | Value 14 | Value 15 | Value 16 | Value 17 | Value 18 | Value 19 | Value 20 | Value 21 | Value 22 | Value 23 | Value 24 | Value 25 | Value 26 | Value 27 | Value 28 | Value 29 | Value 30 | Value 31 | Value 32 | Value 33 | Value 34 | Value 35 | Value 36 | Value 37 | Value 38 | Value 39 | Value 40 | Value 41 | Value 42 | Value 43 | Value 44 | Value 45 | Value 46 | Value 47 | Value 48 | Value 49 | Value 50 | Value 51 | Value 52 | Value 53 | Value 54 | Value 55 | Value 56 | Value 57 | Value 58 | Value 59 | Value 60 | Value 61 | Value 62 | Value 63 | Value 64 | Value 65 | Value 66 | Value 67 | Value 68 | Value 69 | Value 70 | Value 71 | Value 72 | Value 73 | Value 74 | Value 75 | Value 76 | Value 77 | Value 78 | Value 79 | Value 80 | Value 81 | Value 82 | Value 83 | Value 84 | Value 85 | Value 86 | Value 87 | Value 88 | Value 89 | Value 90 | Value 91 | Value 92 | Value 93 | Value 94 | Value 95 | Value 96 | Value 97 | Value 98 | Value 99 | Value 100 | Value 101 | Value 102 | Value 103 | Value 104 | Value 105 | Value 106 | Value 107 | Value 108 | Value 109 | Value 110 | Value 111 | Value 112 | Value 113 | Value 114 | Value 115 | Value 116 | Value 117 | Value 118 | Value 119 | Value 120 | Value 121 | Value 122 | Value 123 | Value 124 | Value 125 | Value 126 | Value 127 | Value 128 | Value 129 | Value 130 | Value 131 | Value 132 | Value 133 | Value 134 | Value 135 | Value 136 | Value 137 | Value 138 | Value 139 | Value 140 | Value 141 | Value 142 | Value 143 | Value 144 | Value 145 | Value 146 | Value 147 | Value 148 | Value 149 | Value 150 | Value 151 | Value 152 | Value 153 | Value 154 | Value 155 | Value 156 | Value 157 | Value 158 | Value 159 | Value 160 | Value 161 | Value 162 | Value 163 | Value 164 | Value 165 | Value 166 | Value 167 | Value 168 | Value 169 | Value 170 | Value 171 | Value 172 | Value 173 | Value 174 | Value 175 | Value 176 | Value 177 | Value 178 | Value 179 | Value 180 | Value 181 | Value 182 | Value 183 | Value 184 | Value 185 | Value 186 | Value 187 | Value 188 | Value 189 | Value 190 | Value 191 | Value 192 | Value 193 | Value 194 | Value 195 | Value 196 | Value 197 | Value 198 | Value 199 | Value 200 |
| x1      | x2      | x3      | y1      | y2      | y3      | T | T | T |
|--------|--------|--------|--------|--------|--------|---|---|---|
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| 0.8182175547794783 | 0.9996791191539316 | 0.5492756302077765 | T | T | T |
| 0.8173554891814481 | 0.7487659964121376 | 0.6881870008219343 | T | T | T |
| 0.9424044427114610 | 0.6587752470778132 | 0.3294033783618361 | T | T | T |
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|          | 0.3210917893623301 | 0.4994414188424790 | 0.8075991399379868 | T | T | T |

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|----------|----------|----------|----------|----------|----------|
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|          | 0.0000000000000000 | 13.5719200000000004 | 0.0000000000000000 | 0.0000000000000000 |
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**Selective dynamics**

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|          |          |          |          |          |          |
|----------|----------|----------|----------|----------|----------|
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| Value 1 | Value 2 | Value 3 | Value 4 | Value 5 | Value 6 | Value 7 | Value 8 | Value 9 |
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| X   | Y   | Width  | Height | T     | T     | T     | T     |
|-----|-----|--------|--------|-------|-------|-------|-------|
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| 0.067929591562079 | 0.5012728803427545 | 0.6573226442781910 | T   | T   | T   | T   |
| 0.1915730724846236 | 0.8411469966764840 | 0.328596988362798 | T   | T   | T   | T   |
| 0.1932771353622324 | 0.6002148842983659 | 0.4695668274924144 | T   | T   | T   | T   |
| 0.1925313165534378 | 0.8503446749745441 | 0.604907273812553 | T   | T   | T   | T   |
| 0.1975956890170917 | 0.5921535131867111 | 0.7495846238943979 | T   | T   | T   | T   |
| 0.0667558639062871 | 0.5001759934919616 | 0.2837923801655630 | T   | T   | T   | T   |
| 0.0674660173875944 | 0.7500857666721990 | 0.4187472135539064 | T   | T   | T   | T   |
| 0.0678407514288192 | 0.9994929559744560 | 0.5488351384235443 | T   | T   | T   | T   |
| 0.0663498954172623 | 0.7498362725294875 | 0.6890224190786434 | T   | T   | T   | T   |
| 0.1923113185866422 | 0.6588298791751686 | 0.3289525380403989 | T   | T   | T   | T   |
| 0.1929363119082524 | 0.8997400996316302 | 0.4691053647740279 | T   | T   | T   | T   |
| 0.1932130284767897 | 0.6506860363054725 | 0.6064279526178734 | T   | T   | T   | T   |
| 0.1975765521589971 | 0.9069659027173651 | 0.7481515239777246 | T   | T   | T   | T   |
| 0.0731563698561030 | 0.7521963774285073 | 0.7924228874663005 | T   | T   | T   | T   |
| 0.3180233029180309 | 0.4996120961609127 | 0.3880168458362084 | T   | T   | T   | T   |
| 0.3188869727549069 | 0.7501500255560143 | 0.5251452023922807 | T   | T   | T   | T   |
| 0.3145462033792799 | 0.5029344487179873 | 0.6612807311675658 | T   | T   | T   | T   |
| 0.4416273103443942 | 0.8410989403708160 | 0.3282298660366744 | T   | T   | T   | T   |
| 0.4428726824470909 | 0.6001956145031845 | 0.4692054954139128 | T   | T   | T   | T   |
| 0.4436359538616918 | 0.8489395465087431 | 0.6082921015973368 | T   | T   | T   | T   |
| 0.4514134450916845 | 0.6208686456313278 | 0.7198436252705763 | T   | T   | T   | T   |
| 0.3167750627625242 | 0.5002511577147906 | 0.2848184137163979 | T   | T   | T   | T   |
| Value1 | Value2 | Value3 | Value4 | Value5 | Value6 | Value7 | Value8 |
|--------|--------|--------|--------|--------|--------|--------|--------|
| 0.3172740641817884 | 0.7503857156409088 | 0.4182039863898878 | T | T | T | T | T |
| 0.3186083276043876 | 0.9984529856408947 | 0.5488735441550026 | T | T | T | T | T |
| 0.3061349185766287 | 0.7609975251257136 | 0.6876627660778001 | T | T | T | T | T |
| 0.4425090263542620 | 0.6588282174452067 | 0.3290235929921385 | T | T | T | T | T |
| 0.4429420300635817 | 0.8996551876490217 | 0.4691533750176175 | T | T | T | T | T |
| 0.4437058443552323 | 0.6521273002317509 | 0.6068849461186518 | T | T | T | T | T |
| 0.4431183429613939 | 0.9076976134937623 | 0.7447827717348620 | T | T | T | T | T |
| 0.3370181350857896 | 0.7383297160649311 | 0.7935931210939621 | T | T | T | T | T |
| 0.5678741408182367 | 0.9995250001640299 | 0.3862113050895847 | T | T | T | T | T |
| 0.5677707431731658 | 0.2496284193377765 | 0.5263200828969243 | T | T | T | T | T |
| 0.5682933972682194 | 0.9989399356057804 | 0.6566808050613032 | T | T | T | T | T |
| 0.6916839860941716 | 0.3410170289503173 | 0.3290409445892716 | T | T | T | T | T |
| 0.6928734366951114 | 0.0998679036954403 | 0.4691693239799840 | T | T | T | T | T |
| 0.6931431488916936 | 0.3493621990067426 | 0.6006578451810175 | T | T | T | T | T |
| 0.7016603184342414 | 0.0900704017083119 | 0.7482130153906835 | T | T | T | T | T |
| 0.5665308371680295 | 0.0000261989508040 | 0.2832141159008302 | T | T | T | T | T |
| 0.5677045053232852 | 0.2496994296856826 | 0.4190943675695305 | T | T | T | T | T |
| 0.5665848786086415 | 0.5009268543187331 | 0.5511745112355989 | T | T | T | T | T |
| 0.5723286918925019 | 0.2361118826430464 | 0.6878084423065315 | T | T | T | T | T |
| 0.6924923606988043 | 0.1587006875842046 | 0.3291179833628201 | T | T | T | T | T |
| 0.6927278409368081 | 0.3998047875138709 | 0.4698682349835429 | T | T | T | T | T |
| 0.6940084299238584 | 0.1487983360833635 | 0.6047022628954702 | T | T | T | T | T |
| 0.6935534367844017 | 0.4075834241138712 | 0.7468533425659628 | T | T | T | T | T |
| 0.5711949130575529 | 0.2479079324383020 | 0.7904705846952622 | T | T | T | T | T |
| 0.8179542392451475 | 0.9995456084365398 | 0.3862886589716896 | T | T | T | T | T |
| 0.8181073842685068 | 0.2497136170852049 | 0.5264824219483646 | T | T | T | T | T |
| 0.8181769204041485 | 0.9985253192461886 | 0.6569228010796317 | T | T | T | T | T |
| x   | y   | z       | t_1   | t_2   | t_3   | t_4   | t_5   | t_6   |
|-----|-----|---------|-------|-------|-------|-------|-------|-------|
| 0.9416182405704520 | 0.3410411996107999 | 0.3288787101922335 | T     | T     | T     | T     |       |
| 0.9429391669509138 | 0.0999582049424829 | 0.4690603738858200 | T     | T     | T     |       |
| 0.9430375701893166 | 0.3500134614641296 | 0.6061332410648297 | T     | T     | T     |       |
| 0.9479492445589921 | 0.0900182280373385 | 0.7470795439266177 | T     | T     | T     |       |
| 0.8164652298924377 | 0.0003184535202701 | 0.2832578012233538 | T     | T     | T     |       |
| 0.8177379607256243 | 0.2499637870268647 | 0.4190978696932508 | T     | T     | T     |       |
| 0.8178498561616255 | 0.500121832669673 | 0.5494407779701285 | T     | T     | T     |       |
| 0.818051184541957 | 0.2490279808837783 | 0.6888251237089881 | T     | T     | T     |       |
| 0.9425509826877287 | 0.1586650671529594 | 0.3291035640166535 | T     | T     | T     |       |
| 0.9432878882177889 | 0.3997298933469368 | 0.4697514789634329 | T     | T     | T     |       |
| 0.9431420748761647 | 0.1492981873468816 | 0.6060094403089153 | T     | T     | T     |       |
| 0.9442011846066253 | 0.4096350196459404 | 0.7461202658026550 | T     | T     | T     |       |
| 0.8228218912727828 | 0.2503871436497722 | 0.7921261196920977 | T     | T     | T     |       |
| 0.5682176972820157 | 0.4995993083935983 | 0.3878413800114531 | T     | T     | T     |       |
| 0.5669779188311808 | 0.7501011449640664 | 0.5251753064091851 | T     | T     | T     |       |
| 0.5745939468915833 | 0.5012684261483745 | 0.6602354057194254 | T     | T     | T     |       |
| 0.6918239543760855 | 0.8411373282523089 | 0.3286199521404285 | T     | T     | T     |       |
| 0.6927685548972209 | 0.6001321763439553 | 0.4693944577305975 | T     | T     | T     |       |
| 0.6945165813783688 | 0.8504393920117381 | 0.6044425870010686 | T     | T     | T     |       |
| 0.6921810838169321 | 0.5920210925618260 | 0.7499824162290888 | T     | T     | T     |       |
| 0.5660277394446782 | 0.5001525023988631 | 0.2847432002237117 | T     | T     | T     |       |
| 0.5682357358885871 | 0.7503546089103349 | 0.4182118117999280 | T     | T     | T     |       |
| 0.5678320927831529 | 0.9985429284315971 | 0.5488479605929921 | T     | T     | T     |       |
| 0.5838219734119645 | 0.7638184070841952 | 0.6878582343363803 | T     | T     | T     |       |
| 0.6925579254636842 | 0.6588041921417154 | 0.3289800885162713 | T     | T     | T     |       |
| 0.6929489467443861 | 0.8996897940384566 | 0.4690898843809315 | T     | T     | T     |       |
| 0.6938112511917033 | 0.6506357054698071 | 0.6059797050213581 | T     | T     | T     |       |
ad-FeO wH

1.000000000000000

13.367000000000009 0.0000000000000000 0.0000000000000000

0.0000000000000000 13.5719200000000004 0.0000000000000000

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Selective dynamics
| Direct          | 0.1935618921876849 | 0.9999998876280370 | 0.3268344764099149 | T  | T  | T   |
|----------------|-------------------|-------------------|-------------------|----|----|-----|
|                | 0.1933064537463780| 0.2499103472351525| 0.4732825317968535| T  | T  | T   |
|                | 0.1943779818067293| 0.4998042147747645| 0.6048390192057976| T  | T  | T   |
|                | 0.1996106707814301| 0.2520729273421254| 0.7483737053093060| T  | T  | T   |
|                | 0.4436186983108943| 0.9998839765123622| 0.3266290575658959| T  | T  | T   |
|                | 0.4432396142535295| 0.2499225748811911| 0.4730074764037518| T  | T  | T   |
|                | 0.4436235053265735| 0.5003038518809462| 0.6064462789267967| T  | T  | T   |
|                | 0.4497024152834659| 0.2513672557864232| 0.7457789897844188| T  | T  | T   |
|                | 0.1914584428196163| 0.4998163509326400| 0.3288357805471260| T  | T  | T   |
|                | 0.1928049141853057| 0.7499977715813684| 0.4720615212038768| T  | T  | T   |
|                | 0.1933827545237575| 0.0002103959431007| 0.6017567365092423| T  | T  | T   |
|                | 0.1919771538027257| 0.7504480358294077| 0.7481594671925753| T  | T  | T   |
|                | 0.4413354003220340| 0.4997282325610963| 0.3291926857586625| T  | T  | T   |
|                | 0.4435515665917009| 0.7499176431790585| 0.4714886143260708| T  | T  | T   |
|                | 0.4437541536137228| 0.9999901625323735| 0.6018901511270135| T  | T  | T   |
|                | 0.4385866175208177| 0.7542159444301132| 0.7365845267749882| T  | T  | T   |
|                | 0.6936275084161372| 0.9999988291880840| 0.3269291082152812| T  | T  | T   |
|                | 0.6935181164474449| 0.2500259710061570| 0.4729704483230041| T  | T  | T   |
|                | 0.6947107235876395| 0.4998896318196621| 0.6022008692654391| T  | T  | T   |
|                | 0.7002992948523756| 0.2501323876264316| 0.7482090848852748| T  | T  | T   |
|                | 0.9436436520163123| 0.00000785854069426| 0.3269720374876003| T  | T  | T   |
|                | 0.9435437690921166| 0.2500300219156493| 0.4731332982845712| T  | T  | T   |
|                | 0.9446258197238606| 0.4998847783227377| 0.6023274211074557| T  | T  | T   |
|                | 0.9500219102613038| 0.2497419963249468| 0.7483688348241295| T  | T  | T   |
|                | 0.6913428160047688| 0.4997718821673537| 0.3278444981332448| T  | T  | T   |
|                | 0.6933715406243246| 0.7499136111953140| 0.4723018568829617| T  | T  | T   |
| 0.6940130442987321 | 1.0000468695488820 | 0.6019532128024305 | T  | T  | T  | T  |
| 0.6938906894147460 | 0.7482618630186878 | 0.746887782789631 | T  | T  | T  | T  |
| 0.9413752399836348 | 0.4998646201831746 | 0.3274990102607163 | T  | T  | T  | T  |
| 0.9431932912584097 | 0.7498749731796737 | 0.4725024836578725 | T  | T  | T  | T  |
| 0.9437356060817452 | 1.0000135029427528 | 0.6025468153376733 | T  | T  | T  | T  |
| 0.9422245869627747 | 0.7501168529927003 | 0.7478059894259548 | T  | T  | T  | T  |
| 0.0675400815872965 | 0.2499398779954157 | 0.3378102728766358 | T  | T  | T  | T  |
| 0.0687568789798950 | 0.4999714901391504 | 0.4681189675249482 | T  | T  | T  | T  |
| 0.0686011675078874 | 0.2499204834577347 | 0.6084076353815612 | T  | T  | T  | T  |
| 0.0707863706700364 | 0.0010600874463009 | 0.7379319081814675 | T  | T  | T  | T  |
| 0.317561814579555 | 0.2498238623490494 | 0.3378559174254793 | T  | T  | T  | T  |
| 0.3185484419651924 | 0.4999323617268976 | 0.4693814978603156 | T  | T  | T  | T  |
| 0.3186078031365101 | 0.2498366261504250 | 0.6081276689418664 | T  | T  | T  | T  |
| 0.319928097825026 | 0.0012740935487997 | 0.7372503532036817 | T  | T  | T  | T  |
| 0.0675534935896262 | 0.7499162037788559 | 0.3369065691877934 | T  | T  | T  | T  |
| 0.0681490070952340 | 1.0000036300368393 | 0.4668455976296199 | T  | T  | T  | T  |
| 0.0683305006158348 | 0.7499720562213018 | 0.6077867983519623 | T  | T  | T  | T  |
| 0.0724872298926814 | 0.5000938018623852 | 0.7383865489115911 | T  | T  | T  | T  |
| 0.3176509761662652 | 0.7499502904778367 | 0.3366367604056467 | T  | T  | T  | T  |
| 0.3182954765218022 | 0.9999050799356213 | 0.4666330003379748 | T  | T  | T  | T  |
| 0.3169615778335474 | 0.7506925517722567 | 0.6056536656292458 | T  | T  | T  | T  |
| 0.3234913749856250 | 0.5014541578917269 | 0.7435429310874856 | T  | T  | T  | T  |
| 0.5675112513625871 | 0.2497927647844226 | 0.3377412608649557 | T  | T  | T  | T  |
| 0.5680644838330159 | 0.4999052214575437 | 0.4684350769559482 | T  | T  | T  | T  |
| 0.5690045292617241 | 0.2499091074243641 | 0.6076451582331034 | T  | T  | T  | T  |
| 0.5712592918050591 | 0.0032075529213395 | 0.7372734361691904 | T  | T  | T  | T  |
| 0.8176058930382819 | 0.2499986927628257 | 0.3377170689734471 | T  | T  | T  | T  |
| x-value  | y-value  | z-value  | T | T | T     |
|---------|---------|---------|---|---|-------|
| 0.8184760717884010 | 0.4999408091998924 | 0.4672743775153370 | T | T | T     |
| 0.8188723341378109 | 0.2498838947730855 | 0.6081009484199908 | T | T | T     |
| 0.8205290614678712 | 0.9986094921373863 | 0.7380820471926568 | T | T | T     |
| 0.5677188833295409 | 0.7497341572538313 | 0.3366902503651838 | T | T | T     |
| 0.5683668276406787 | 0.9999779127584495 | 0.4666955468284897 | T | T | T     |
| 0.5696918676104739 | 0.7502249670814172 | 0.6071201740385349 | T | T | T     |
| 0.5737149592599166 | 0.4994276311822126 | 0.7380292290828453 | T | T | T     |
| 0.8177365355145267 | 0.7500860743925917 | 0.3369613922292429 | T | T | T     |
| 0.8183877821181388 | 0.9999654122343524 | 0.4669097066562353 | T | T | T     |
| 0.8195619425852837 | 0.7502396580770181 | 0.6076462544375073 | T | T | T     |
| 0.8236521604436029 | 0.4988844346663966 | 0.7370682192018341 | T | T | T     |
| 0.4777838699161492 | 0.6146122250526977 | 0.8221709095593013 | T | T | T     |
| 0.0686064004556665 | 0.9998598974253110 | 0.3857453939724617 | T | T | T     |
| 0.0683884254570674 | 0.2495395077241291 | 0.5268475171785939 | T | T | T     |
| 0.0692705913901760 | 0.9989444160803914 | 0.6564326021797025 | T | T | T     |
| 0.191460958519075 | 0.3410132908430490 | 0.329416651851717 | T | T | T     |
| 0.1933101872519057 | 0.1000053744895657 | 0.4689094375979941 | T | T | T     |
| 0.1938313062968973 | 0.3497877201718658 | 0.6067996275839936 | T | T | T     |
| 0.1995884909418076 | 0.0925680754553055 | 0.7467631121876448 | T | T | T     |
| 0.0685500046447819 | 0.0005552926583676 | 0.2826499461550975 | T | T | T     |
| 0.0684072155699889 | 0.2503257536685151 | 0.4192525617872360 | T | T | T     |
| 0.0699552095653649 | 0.5001932438016777 | 0.5494293742132930 | T | T | T     |
| 0.0679613824113800 | 0.2488976008698039 | 0.6891673230889228 | T | T | T     |
| 0.1937257479329166 | 0.1587131997188615 | 0.3289107991374573 | T | T | T     |
| 0.1937784043759868 | 0.3998013910319063 | 0.4709249372146663 | T | T | T     |
| 0.1934026761973632 | 0.1495157847712477 | 0.6054582335830255 | T | T | T     |
| 0.1949607344276172 | 0.4076654945777800 | 0.7464223770179838 | T | T | T     |
|        |        |        |        |        |        |        |        |        |
|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| 0.0766083427792201 | 0.2474696918526656 | 0.7927433219061579 | T | T | T | T | T | T |
| 0.3186791048246521  | 0.9997466405809059  | 0.3855998656798250  | T | T | T | T | T | T |
| 0.3185882300269741  | 0.2499119952671871  | 0.5267152754747411  | T | T | T | T | T | T |
| 0.3189023406725146  | -0.0003670155691109 | 0.6558544210532649  | T | T | T | T | T | T |
| 0.4414704216876286  | 0.3408761112405628  | 0.3292989410550763  | T | T | T | T | T | T |
| 0.4433716211415423  | 0.0999769158117480  | 0.4687097599057438  | T | T | T | T | T | T |
| 0.4436077006236281  | 0.3500375467719237  | 0.607187862118810  | T | T | T | T | T | T |
| 0.4483120595619420  | 0.0901294972645494  | 0.7481246890496103  | T | T | T | T | T | T |
| 0.3185309152640310  | 0.0001308548258509  | 0.2825264309136059  | T | T | T | T | T | T |
| 0.3180684250427031  | 0.2500174537838394  | 0.4192762226456539  | T | T | T | T | T | T |
| 0.3198742514611067  | 0.5009539418166340  | 0.5513560274305892  | T | T | T | T | T | T |
| 0.3185519920586435  | 0.2452008034153013  | 0.688855189722939    | T | T | T | T | T | T |
| 0.4436418942774210  | 0.1585151563725272  | 0.3289466104515963  | T | T | T | T | T | T |
| 0.4431864065933631  | 0.3997404895980865  | 0.4703622249441017  | T | T | T | T | T | T |
| 0.4437449718630881  | 0.1494471361843518  | 0.605272898392355    | T | T | T | T | T | T |
| 0.4557063135666616  | 0.4059539513360828  | 0.7371626747014318   | T | T | T | T | T | T |
| 0.3283460149261850  | 0.2566774726160092  | 0.7917659922702071   | T | T | T | T | T | T |
| 0.0685948784952250  | 0.4997423535632453  | 0.3870256905891246   | T | T | T | T | T | T |
| 0.0681315189154723  | 0.7497117832814595  | 0.5259647381185518   | T | T | T | T | T | T |
| 0.0677929390007101  | 0.5011491746202887  | 0.6566488200755670   | T | T | T | T | T | T |
| 0.1942874486199718  | 0.8411634182954757  | 0.3279341549618160   | T | T | T | T | T | T |
| 0.1937620695264970  | 0.6002463783442358  | 0.4696992988725551   | T | T | T | T | T | T |
| 0.1923588022532259  | 0.8507504960341151  | 0.603422508583665    | T | T | T | T | T | T |
| 0.1894650940614836  | 0.5948230123159902  | 0.7463003549071809   | T | T | T | T | T | T |
| 0.0661240016273626  | 0.4998140162384544  | 0.2839710958565071   | T | T | T | T | T | T |
| 0.0678434573029561  | 0.7498221348616436  | 0.4183141777480132   | T | T | T | T | T | T |
| 0.0678717794613256  | 0.0005512059235764  | 0.5483496906258375   | T | T | T | T | T | T |
|          |          |          |          |          |          |          |
|----------|----------|----------|----------|----------|----------|----------|
| 0.0668245357638345 | 0.7516197460295789 | 0.6886319629881177 | T | T | T | T |
| 0.190865862628508  | 0.6587412157450047  | 0.3288964403333605  | T | T | T | T |
| 0.1931488064967637  | 0.8998173320883267  | 0.4685540491788466  | T | T | T | T |
| 0.1934518773152904  | 0.6500491971793129  | 0.6055204653498386  | T | T | T | T |
| 0.1922500985531176  | 0.9100182620646411  | 0.7478147640924876  | T | T | T | T |
| 0.0668112682701950  | 0.7536339543415800  | 0.7921231419553721  | T | T | T | T |
| 0.3183932161288525  | 0.4994209842151503  | 0.3880234237225632  | T | T | T | T |
| 0.3192029490902649  | 0.7500267128911887  | 0.5249799055479001  | T | T | T | T |
| 0.3163453391087486  | 0.4987631026703865  | 0.6610615280290789  | T | T | T | T |
| 0.4445399813182154  | 0.8409245940722189  | 0.3273281366857621  | T | T | T | T |
| 0.4432135503546061  | 0.6003143492923115  | 0.4692700623285056  | T | T | T | T |
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| 0.4480499948769975  | 0.6048006504127786  | 0.7263319073895623  | T | T | T | T |
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| 0.3092126642689997  | 0.7588800668624421  | 0.6860244940382468  | T | T | T | T |
| 0.4410246881748981  | 0.6585900156277018  | 0.3289763127384651  | T | T | T | T |
| 0.4434926880479275  | 0.8997445079579820  | 0.4683936065759211  | T | T | T | T |
| 0.4439784514742536  | 0.6515375016060981  | 0.607425297287827  | T | T | T | T |
| 0.4431365625970359  | 0.9070982131732443  | 0.7437636657794744  | T | T | T | T |
| 0.3243199292415339  | 0.7531463380352527  | 0.7892278118588908  | T | T | T | T |
| 0.5686343562152734  | 0.9997133262119200  | 0.3856407603258583  | T | T | T | T |
| 0.5683301812944118  | 0.2498934719824014  | 0.5263684696939820  | T | T | T | T |
| 0.5690025639252042  | 1.0003429025602963  | 0.6560562372814974  | T | T | T | T |
| 0.6914944318510818  | 0.3410154291809898  | 0.3292349882707317  | T | T | T | T |
| 0.6932825244351758  | 0.1000524053610036  | 0.4689128341598360  | T | T | T | T |
| X          | Y          | Z          | A  | B    | C  | D    | E  | F  |
|------------|------------|------------|----|------|----|------|----|----|
| 0.69420771 | 0.34957963 | 1164075    | T  | T    | T  | T    |    |    |
| 0.70143027 | 0.09001094 | 67561978   | T  | T    | T  | T    |    |    |
| 0.56874321 | 0.00300544 | 3829967   | T  | T    | T  | T    |    |    |
| 0.56821291 | 0.25009980 | 21081587   | T  | T    | T  | T    |    |    |
| 0.56727854 | 0.50139667 | 97688204   | T  | T    | T  | T    |    |    |
| 0.57107405 | 0.24375189 | 81781474   | T  | T    | T  | T    |    |    |
| 0.69369572 | 0.15872083 | 304962673  | T  | T    | T  | T    |    |    |
| 0.69333171 | 0.39986689 | 7844601    | T  | T    | T  | T    |    |    |
| 0.69418630 | 0.14927532 | 84634096   | T  | T    | T  | T    |    |    |
| 0.70425762 | 0.40797085 | 91581488   | T  | T    | T  | T    |    |    |
| 0.57991108 | 0.24850483 | 31860314   | T  | T    | T  | T    |    |    |
| 0.81855418 | 0.99974099 | 48949597   | T  | T    | T  | T    |    |    |
| 0.81877913 | 0.24942789 | 70115872   | T  | T    | T  | T    |    |    |
| 0.81822998 | 0.99854578 | 888150213  | T  | T    | T  | T    |    |    |
| 0.94153351 | 0.34119312 | 67115729   | T  | T    | T  | T    |    |    |
| 0.94323667 | 0.10013448 | 855867818  | T  | T    | T  | T    |    |    |
| 0.94384906 | 0.34983552 | 65026166   | T  | T    | T  | T    |    |    |
| 0.94983231 | 0.09089929 | 05928381   | T  | T    | T  | T    |    |    |
| 0.81866600 | 0.00024714 | 473315030  | T  | T    | T  | T    |    |    |
| 0.81842646 | 0.25039089 | 81982043   | T  | T    | T  | T    |    |    |
| 0.81914993 | 0.50068431 | 112429993  | T  | T    | T  | T    |    |    |
| 0.81881392 | 0.24930454 | 050177777  | T  | T    | T  | T    |    |    |
| 0.94366481 | 0.15882247 | 62849826   | T  | T    | T  | T    |    |    |
| 0.94368092 | 0.39986977 | 06114624   | T  | T    | T  | T    |    |    |
| 0.94350817 | 0.14938471 | 69034022   | T  | T    | T  | T    |    |    |
| 0.95078138 | 0.40813109 | 16707711   | T  | T    | T  | T    |    |    |
| 0.82691386 | 0.24840857 | 770618583  | T  | T    | T  | T    |    |    |
|    |    |    |    |    |    |    |    |    |    |    |    |    |    |
|----|----|----|----|----|----|----|----|----|----|----|----|----|----|
| 0.5684119691957459 | 0.4995299192105289 | 0.3872692491185675 | T | T | T |
| 0.5678007819458764 | 0.7500083905336012 | 0.5259472016530430 | T | T | T |
| 0.5734474065955593 | 0.4986044365234159 | 0.6559807086370940 | T | T | T |
| 0.6944438234828262 | 0.8410709315882067 | 0.3279115742783641 | T | T | T |
| 0.6932369840331083 | 0.6002201459972580 | 0.4692025042857798 | T | T | T |
| 0.693624535497361 | 0.8500865288370089 | 0.6062946262282419 | T | T | T |
| 0.6971761374174851 | 0.593837954539548 | 0.7418430068526736 | T | T | T |
| 0.5651438584620684 | 0.4998474461094043 | 0.2843434578254682 | T | T | T |
| 0.5685704117314988 | 0.7501318951643192 | 0.4181568980756243 | T | T | T |
| 0.5686045216558646 | 0.9989847984477002 | 0.5483264522120532 | T | T | T |
| 0.5747613102657023 | 0.7572843328831280 | 0.6908131873639356 | T | T | T |
| 0.6910901674931792 | 0.6586311694462185 | 0.3284863348457633 | T | T | T |
| 0.6932954095856750 | 0.8997424928103286 | 0.4687837941185688 | T | T | T |
| 0.6938132861245845 | 0.6509288707953189 | 0.6067429942931245 | T | T | T |
| 0.6867546350461139 | 0.9063763755356505 | 0.7493817275599172 | T | T | T |
| 0.5588497395186167 | 0.7267084770475790 | 0.7984044965146657 | T | T | T |
| 0.8185270448160947 | 0.4998598741052648 | 0.3863126089697059 | T | T | T |
| 0.8179780882417345 | 0.7501364517316432 | 0.5261585125731751 | T | T | T |
| 0.820532333051825 | 0.4998420413000355 | 0.6555683899365615 | T | T | T |
| 0.9445487776427143 | 0.8412512060048922 | 0.3280951282130787 | T | T | T |
| 0.9435095142668617 | 0.6001239536409405 | 0.4689083244717572 | T | T | T |
| 0.9436693024535308 | 0.8505008187733774 | 0.6054202476978668 | T | T | T |
| 0.9425277389573929 | 0.5921470567161212 | 0.7473642081982245 | T | T | T |
| 0.8155118961444628 | 0.4994506622755490 | 0.2833674455095520 | T | T | T |
| 0.8182472720508048 | 0.7499410288825282 | 0.4184113582939726 | T | T | T |
| 0.8189180482728036 | 0.9995969441895727 | 0.5485164521502958 | T | T | T |
| 0.8217517871779569 | 0.7529554828893215 | 0.6887553774088090 | T | T | T |
Supplementary Discussion 1: Material characterization.

IFONFs almost have a constant Fe content of ~19 wt% in ICP-MS, whereas F content increase from 6.76 to 16.32 at% and the surface O content decrease significantly from 45.62 to 30.38 at% in XPS (Supplementary Table 1), suggesting that O atoms are partial substituted by F atoms with fluorination processing.

Note that, as $T_{\text{fluorinated}}$ prolonged from 15 to 90 min, the Fe 2$p_{3/2}$ and Fe 2$p_{1/2}$ peaks both exhibit positive shift to higher binding energy, confirming the existence of strong electronic interactions between FeF$_2$ and Fe$_2$O$_3$ in the hybrid (Supplementary Fig. 5b). While, the observed C peaks should arise from the residual organic electrolyte in the nanoporous layer (Supplementary Fig. 6). Therefore, the above results confirm the successful transformation of Fe-oxide into iron fluoride-oxide.

These results prove that fluorination reaction with NH$_4$F is a facile pathway to successfully convert iron compounds including Fe$_2$O$_3$ and FeO(OH) into FeF$_2$. Such a 3D nanoporous filmed and interconnected hybrid with integrated advantages of high surface area and short electron-transfer pathways may facilitate electrochemical reactions. Moreover, the fluorination method reported here is much easier and faster than other reported iron fluoride preparation methods because of no requirement for highly toxic materials or high-temperature growth process.

As $T_{\text{fluorinated}}$ prolonging, FeF$_2$ phase perfection increasing and FeF$_2$-F$_2$O$_3$ interfaces reducing occur simultaneously as more Fe$_2$O$_3$ nanodomains transfer into FeF$_2$ phase, which result in a much reduced defect state. Thereby, defect states including interphase boundary and phase junction could reach top amount with medium $T_{\text{fluorinated}}$ (i.e., 45 min).

In Supplementary Fig. 24, Fe$_2$O$_3$ (400) surface with iron termination is combined with FeF$_2$ (101) surface with fluorine termination in FeF$_2$-F$_2$O$_3$ hybrid, and different FeF$_2$ (101) surfaces with fluorine termination can be got by cutting with different depths of bulk FeF$_2$. All of the above reasons will induce the formation of interfaces between FeF$_2$ and Fe$_2$O$_3$, which could significantly increase the exposure of active edge sites for heterocatalyst. In general, the heterogeneous iron fluoride-oxide nanoporous films were prepared by controlling the fluorination process. Rational $T_{\text{fluorinated}}$ is the prerequisite for the formation of defect-enriched IFONFs heterostructure. With medium $T_{\text{fluorinated}}$, the fluorination process keeps insufficient, remaining Fe-O bonds inherited from the anodized Fe-oxide, realizing partial conversion of nanoporous Fe-oxide to iron fluoride-oxide through reaction with fluorine vapor. Thus, the heterogeneous nanocomposites
possess embedded disorder phases in crystalline lattices, containing numerous scattered defects such as interphase boundaries, stacking faults, \( V_O \) and dislocations on the surfaces/interface. The defect-enriched architectures benefit for the hybrids to catalytically evolve \( H_2 \) and \( O_2 \) as they expose more interior sites derived from basal-plane/edge activity\(^{47}\).

**Supplementary Discussion 2: Electrochemical characterization**

We hypothesize that the open and porous heterostructures of IFONFs-45 with numerous defect states and high electrical conductivity facilitate exposure of more active basal-plane/edge sites and provide more pathways for ion and mass transport. Thus, the synergistic effect from dense interior sites at the iron fluoride-oxide hybrid surface/interface endows the heterocatalyst with the significant improvement for HER kinetics.

The defect-rich feature can ensure an isotropic electron transport from Fe foil substrate to iron fluoride-oxide edges and significantly decrease the resistance for traversed layers. In addition, the 3D nanoporous filmed heterostructure promotes the release of gas bubbles, enhancing the contact between electrolyte and active sites.

Although Pt and RuO\(_2\) are well recognized as among the most efficient catalysts to generate \( H_2 \) and \( O_2 \), respectively, they cannot perform any bifunctional activity due to the detrimental catalyst deactivation caused by either oxidation of Pt or reduction of RuO\(_2\). The mixed phases of iron fluoride-oxide in IFONFs work for \( H_2 \) and \( O_2 \) generation catalysis during cathodic and anodic sweeps. And the highly porous morphology enhances the HER/OER activities by affording abundant active sites in an extremely low loading mass.

Given the above, the FeF\(_2\)-Fe\(_2\)O\(_3\) direct bonding heterojunctions are successfully obtained with anodization/fluorination process. The surface contact region between the individual Fe\(_2\)O\(_3\) and FeF\(_2\) phases, as well as the synergetic effect of both rich active sites and good conductivity of nanoporous heterostructure lead to remarkably improved activity for electrocatalysis.

On the whole, the IFONFs delivers superior catalytic activity, which benefits from synergistic effects: unique 3D nanoporous structure with numerous defect states that ensures the sufficient exposure and better utilization of electroactive sites, and facilitates electrolyte penetration/diffusion; strong interfacial coupling and interface reconstruction between Fe\(_2\)O\(_3\) and grafted FeF\(_2\) by forming Fe–F bonds, which results in the charge redistribution between the Fe\(_2\)O\(_3\) and FeF\(_2\), and thus lowers the adsorption energy of the reactant and product; together with highly conductive support of Fe foil for efficient charge transfer.

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