

Supporting information

Structured domain knowledge enables trustworthy materials science question-answering with large language models

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| | |
|-------------------------|---|
| Paragraph type | <ul style="list-style-type: none"> System Electrodes for water electrolysis are fabricated through processes involving material deposition, structuring, and assembly. Performance The electrochemical properties and overall performance of water electrolysis electrodes are evaluated through analyses such as activity tests, stability assessments, and efficiency measurements. Synthesis Materials such as catalysts are synthesized through chemical or physical processes, distinct from electrode fabrication, to obtain the desired composition and structure. Others Paragraph types different from those defined above. |
| Synthesis method | <ul style="list-style-type: none"> Vapor-phase reactants are converted into a gaseous state and deposited on the surface of a solid through chemical or physical processes. Solid-phase Using solid-state reactants, processes such as heat treatment and mixing are employed to induce direct reactions between the reactants. Hydro/Solvothermal Input materials are dissolved into a liquid solution, which is then subjected to a high-temperature, high-pressure environment. Precipitation Input materials are dissolved into a liquid solution, and precipitate is obtained through processes such as pH adjustment, centrifugation, and heating. Electrodeposition A two or three electrode system is operated within a solution containing an electrolyte, and when a current or voltage is applied, deposition occurs on the working electrode. Sol-gel Input materials are dissolved into a liquid solution, which is kept stirred or heated until a gel is formed, and then the gel is dried and annealed. Others Synthesis methods different from those defined above. |
| Synthesis entity | <ul style="list-style-type: none"> Target The primary material ultimately synthesized, representing the final target of the synthesis process rather than an intermediate. Precursor Metal-based starting compounds or reagents that are utilized to obtain the target material during synthesis. Solvent The base liquid in which precursors are dissolved, serving as the reaction medium throughout the synthesis process. Additive A substance, typically dissolved in the solvent, that optimizes synthesis conditions and influences the structure or properties of the target material. Substrate A base material on which synthesis occurs, or a supporting material that provides structural stability for the synthesized product. |

Supplementary Fig 1. Descriptions of categories and entities used in the paper's preprocessing stages. Most descriptions were based on commonly established criteria, with target and precursor entities described using more stringent standards than their conventional characterizations.

Paragraph classification prompt



Instruction

As a catalyst expert in materials science, classify each paragraph into one of the following four paragraph types: 'synthesis', 'system', 'performance' and 'others'. Each paragraph should belong to only one category. Always include a sentence in the format of 'the answer is paragraph type' at the end of the answer.



Example Q&A

PD-Co(OH)2/CC was prepared as follows. In a typical synthesis, the carbon cloth (CC) was cleaned by sonication sequentially in water, ethanol, and acetone for 10 min each and, ... After the deposition, the coated carbon cloth PD-Co(OH)2/CC was rinsed first with water, ethanol and then dried in a vacuum oven at 60 °C for 2 h.

Let's work this out in a step by step way to be sure we have the right answer. The paragraph describes the detailed procedure for preparing PD-Co(OH)2/CC, ... Therefore, the answer is synthesis.



Test Q

The OER performance of Cu(OH)2/CF, CoNiCu-MOF@Cu2O/CF, and CoNiCu-LDH@CuO/CF was estimated by LSV and compared with that of IrO2/CF. ... indicating that pre-synthesizing MOF plays a crucial role in building LDH with improved performance.

Named entity recognition prompt



Instruction

As a catalyst synthesis expert in materials science, label each synthesis entity related to hydrothermal or solvothermal reactions in the given paragraph as one of the following five entity types: 'Solvent', 'Precursor', 'Target', 'Additive' and 'Substrate'. First, identify and extract the primary 'Target' material described in a paragraph. Then, identify and extract the 'Precursor', 'Solvent', 'Additive' and 'Substrate' used in the synthesis of the 'Target' material. The 'Precursor' refers only to a metal precursor that provides a metal elemental source to the 'Target'. Each synthesis entity should belong to only one entity type. Always use the answer format: "{entity type: 'synthesis entity', 'molecular formula', 'metal components'}". If 'molecular formula' is ambiguous or unknown, use 'synthesis entity' as the 'molecular formula'. The 'molecular formula' must represent the complete chemical composition showing all atoms in a compound, not using abbreviated notations such as "acac" (acetylacetonate) or any other chemical shorthand. It is essential to display the exact atomic composition without any abbreviated functional groups or ligands. If the paragraph does not include synthesis entity, the entity in the response should be 'None'.



Example Q&A

The Ni6MnO8 microflower was prepared by a simple solvothermal reaction. Primarily, DMF (30 mL) and acetone (30 mL) were mixed as solution A. ... The Ni6MnO8 with a microflower structure was obtained and denoted as NMO-MF. The synthesis of the Ni6MnO8 hollow sphere (NMO-HS) was analogous to that of NMO-MF but without addition of graphene oxide.

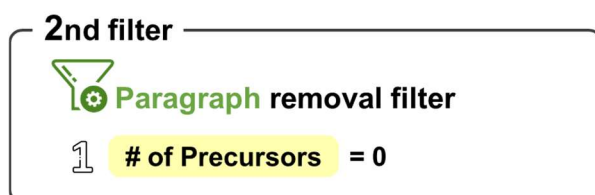
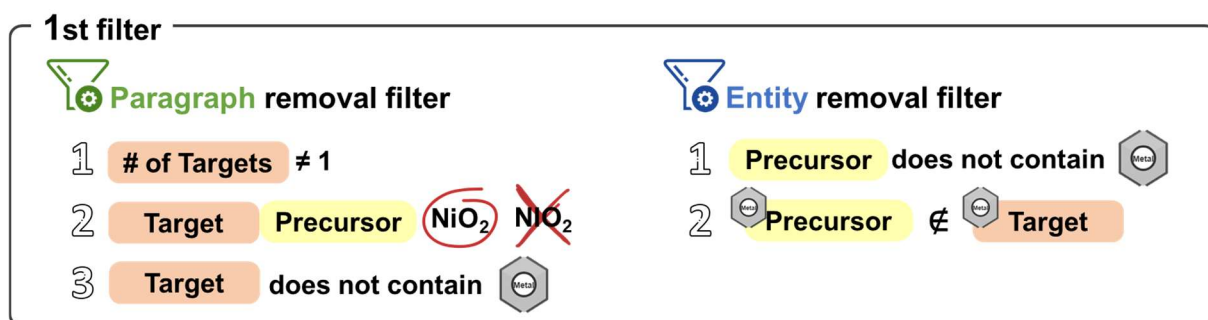
{'TARGET': 'Ni6MnO8', 'Ni6MnO8', 'Ni, Mn'}, {'SOLVENT': 'DMF', 'C3H7NO', 'None'}, {'SOLVENT': 'acetone', 'C3H6O', 'None'}, {'PRECURSOR': 'Ni(NO3)2·6H2O', 'Ni(NO3)2·6H2O', 'Ni'}, ..., {'ADDITIVE': 'graphene oxide', '(C2OH)n', 'None'}




Test Q

In a typical synthesis process, Ni substituted MnCo2O4 (Mn1-xNixCo2O4 with x = 0, 0.2, 0.4, 0.6, 0.8 and 1) on reduced graphene oxide was prepared by facile hydrothermal process, ... Finally, it was dried at 60 °C for 12 h and calcined at 350 °C for 2 h in an Ar atmosphere.


Supplementary Fig 2. GPT prompt design for classification and named entity recognition tasks. For the classification stage, which involves a relatively simple task of classifying large paragraphs based on the overall flow of the document, general instruction prompts were used to make it easily applicable when performing classification in other domains. However, for the NER stage, which involves complex named entity recognition that first identifies main targets and then extracts only entities related to those targets, specialized prompts were used with detailed protocols and direct inclusion of entity definitions tailored specifically to this task. Chain-of-Thought prompting was used in the classification stages, which can be seen in the example answer sections marked in red. For the NER stage, three output formats were defined to apply output filters, as marked in red in the example answers. The NER prompt also includes a normalization step that converts material names to their molecular formula representations (e.g., 'DMF' → 'C3H7NO', 'acetone' → 'C3H6O') to ensure consistency across different naming conventions."



Supplementary Fig 3. Rule-based Filtering System for Named Entity Recognition Results from GPT. The system is divided into two types of filters: filters that remove entire paragraphs and filters that remove only specific entities. The filtering process consists of two stages total. The filters were designed to identify cases where defined target and precursor entities cannot appear together. Filtering was performed based on element capitalization patterns, the number of target entities, and the presence of metal elements.

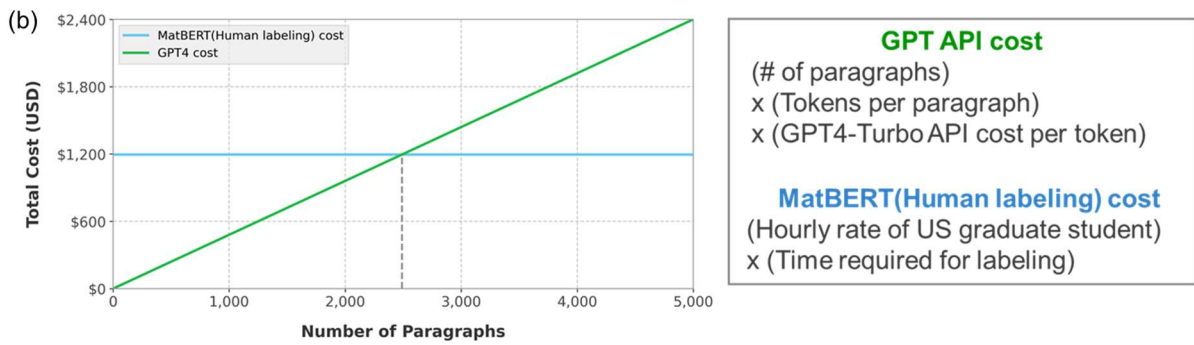
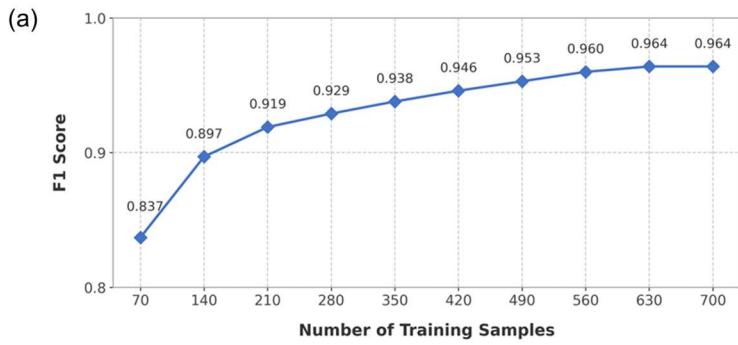
 **Synthesis paragraph**

2 mmol of **Precursor 1** and 1 mmol of **Precursor 2** were completely dissolved in 30 mL of **Solvent 1**. Then, 8 mmol of **Additive 1** and 12 mmol of **Additive 2** were added to the above solution with vigorous stirring. After 30 min, the resulting solution and a piece of **Substrate 1** were transferred into a Teflon-lined stainless-steel autoclave (50 mL) and heated at 120 °C for 800 min. After cooling down, the **Target 1** was obtained and rinsed with deionized water. A similar method as described above was used for the preparation of **Target 2 and 3** where x represents the moles of Co in the original reaction solution. The loading amount of catalysts on **Substrate 2** was calculated as 1.02–1.27 mg cm⁻². To study the effect of reaction time on the electrocatalytic performance of catalysts, we prepared **Target 1** under different reaction times, such as 400, 1200, and 1600 min. In addition, **Target 4** and **Target 5** were synthesized under the same conditions as **Target 1**, except that **Precursor 3** and **Precursor 4** were used, respectively. Note that the total molar quantity of metal ions was 3 mmol.

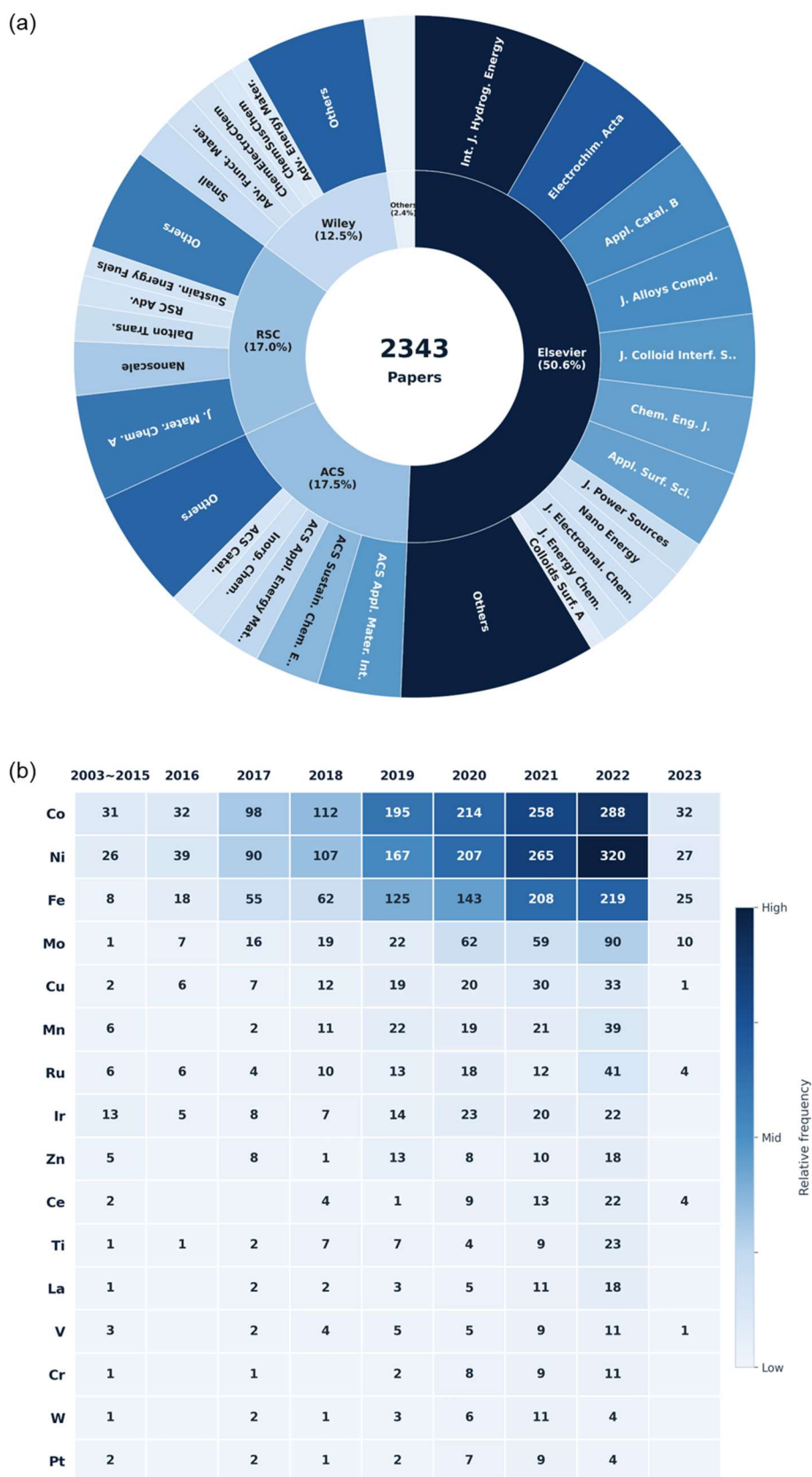
 **Extracted entities**

Target: {Target 1}
Precursor: {Precursor 1, Precursor 2}
Solvent: {Solvent 1}
Additive: {Additive 1, Additive 2}
Substrate: {Substrate 1}


Supplementary Fig 4. Example of relational named entity recognition. Unlike standard NER that considers only word-level features, this task requires contextual understanding to extract only the entities marked in red that are relevant to the main target in a synthetic paragraph.



Supplementary Fig 5. Performance Convergence and Cost-Efficiency Analysis of MatBERT vs. GPT-4 for Paragraph Classification. (a) Classification performance of MatBERT as a function of training sample size for synthesis method classification. The results demonstrate that MatBERT’s performance converges to a level comparable with GPT-4 as the number of training samples increases, identifying the optimal data volume required for high-accuracy classification. (b) Cost comparison between MatBERT and GPT-4 based on classification volume. For the cost-benefit analysis, GPT-4 expenses were calculated using standard API pricing, while MatBERT costs were estimated at approximately \$20 per hour (based on U.S. graduate student wages for manual labeling). Assuming an average manual labeling speed of 1 minute per paragraph, MatBERT becomes more cost-effective than GPT-4 for workloads exceeding approximately 2,500 paragraphs.




Supplementary Fig 6. Statistical overview of the structured database for water-splitting catalysis. (a) Distribution of 2,343 papers across major publishers and journals, showing the diversity of data sources. (b) Heatmap of research frequency by target metal elements and publication year (2003–2023), representing the broad temporal and material coverage of the database.

 — **Single-retrieval condition query**

Easy Extraction Retrieval

What is the DOI of the paper that

1. grew $\text{Fe}(\text{OH})_3$ on $\text{Co}(\text{OH})\text{F}/\text{Ni}(\text{OH})_2$ nanosheets through interfacial hydrolysis?

 — **Multiple-retrieval condition query**

Difficult Extraction Retrieval

What is the DOI of the paper that

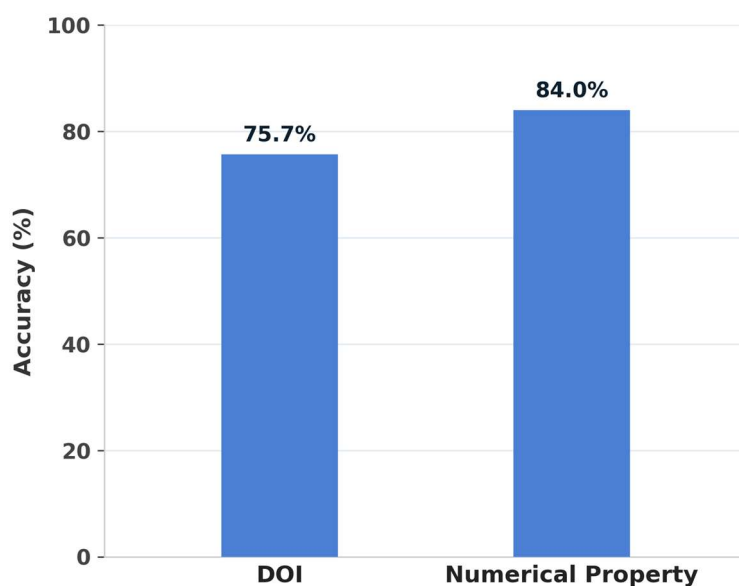
1. grew $\text{Fe}(\text{OH})_3$ on $\text{Co}(\text{OH})\text{F}/\text{Ni}(\text{OH})_2$ nanosheets through interfacial hydrolysis, and

2. elucidated the activation mechanism through in-situ analysis methods?

Supplementary Fig 7. Examples of query types for quantitative evaluation in water-splitting Q/A. Difficulty levels were adjusted based on the number of search conditions highlighted in red, ranging from the easiest problems with a single condition to more challenging problems with multiple conditions to diversify the problem difficulty.

| | C-RAG | QR-RAG |
|--|-------|--------|
| <p>Original query What is the doi of the paper that investigates Ni_2P nanocrystal confinement within NSG for bifunctional catalysis, validated by TEM imaging and long-term overall water splitting data in neutral pH?</p> <p>Reformulated query 1. Ni_2P nanocrystal confinement within NSG for bifunctional catalysis 2. Validation by TEM imaging and long-term overall water-splitting performance at neutral pH</p> | X | O |
| <p>Original query What is the doi of the paper that attributes amorphization-induced OER enhancement in $\text{CoOOH}/\text{W18O49}$ to structural disorder shown in Raman spectra and lowered Tafel slope values?</p> <p>Reformulated query 1. Amorphization-induced OER enhancement in $\text{CoOOH}/\text{W18O49}$ 2. Attribution to structural disorder evidenced by Raman spectra 3. Lowered Tafel slope values supporting the mechanism</p> | X | O |
| <p>Original query What is the doi of the paper that employs electron-paramagnetic resonance to link oxygen-vacancy-rich amorphous NiFe-Pi to accelerated redox cycling of Ni during water oxidation over hundreds of hours?</p> <p>Reformulated query 1. Use of electron-paramagnetic resonance (EPR) to study materials 2. Study of oxygen-vacancy-rich amorphous NiFe-Pi catalyst 3. Investigation of long-term water oxidation stability over hundreds of hours</p> | X | O |

Supplementary Fig 8. Effect of query reformulation on Multi-retrieval condition Q/A. When a question involves multiple conditions, it often becomes a difficult question for retrieval because directly using the entire query diminishes the influence of the key terms that uniquely identify relevant papers, thereby lowering retrieval accuracy. In such cases, the query reformulation process ensures that only the essential components are used for retrieval, mitigating the problems that occur when the full query is applied.



Supplementary Fig 9. Comparison of DOI identification and numerical property extraction accuracy. Accuracy comparison between DOI identification (n=202) and numerical property extraction (n=50) tasks using QR-RAG with structured JSON database and LLaMA 3.3-70B.

Original query

What is the DOI of the paper that presents a strategy for tuning surface energy density of non-stoichiometric perovskite by creating surface defects through a colloidal template strategy?

Paragraph1

...PBC is **decorated** with... **amorphous**... catalyst displays the **best OER activity**... even relative to its **crystalline... counterpart**, owing to the **larger electrolyte-catalyst contact area**...

Paragraph2

...promoting the **OER activity** for **perovskite**... by crystal phase engineering... breaking long-range chemical bonding through **amorphization**... **amorphous** structure... 9-fold increase... compared to **single crystalline**...

Paragraph3

...**amorphization** of materials is also a way to improve **electrocatalytic activity**. **Amorphous** materials are rich in **defects**... better **OER performance** than **amorphous** Co₃O₄ formed by surface oxidation...

Paragraph4

Heterogeneous interface construction... between **amorphous** IrO_x and **crystalline** LaCO₃OH... presents excellent **OER activity**...

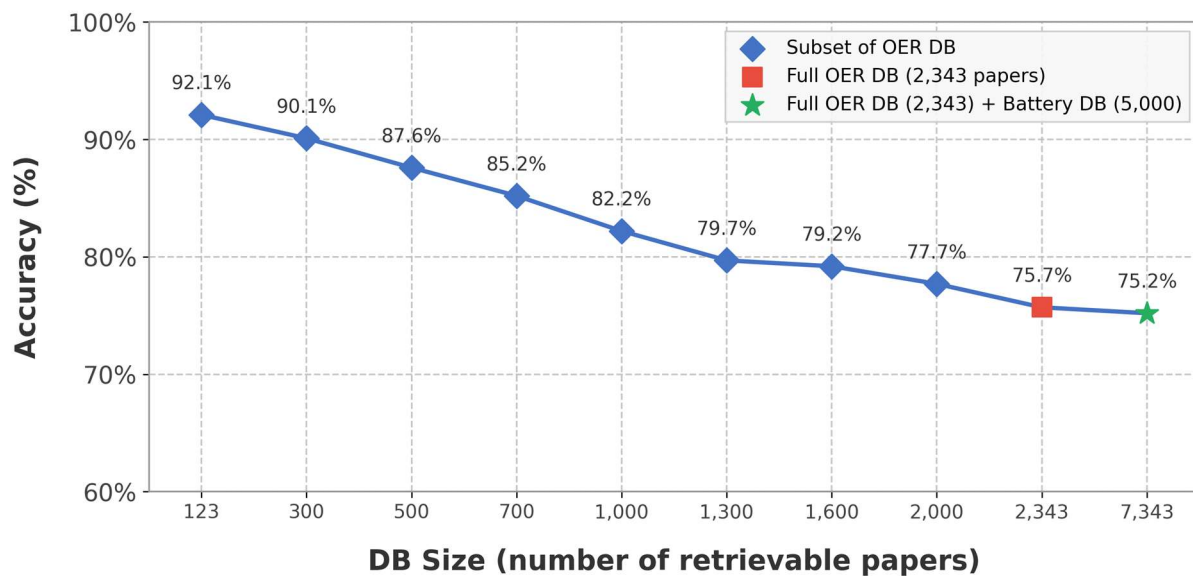
Paragraph5

...construction of OER-induced **crystalline-amorphous combinations**... **perovskite** phases... nano-sized **crystalline-amorphous** combination... top-level performance... **solid-liquid contact**...

Answer

The DOI of the paper that investigates how crystallinity affects the interface between catalyst and electrolyte, demonstrating that amorphous decoration on a perovskite backbone provides superior activity through enhanced contact area compared to crystalline counterparts, is <https://doi.org/10.1002/celc.201600718>. ✓

Supplementary Fig 10. Case study of precise answer identification within high-similarity retrieval scenarios using QR-RAG. This figure presents a representative case where the LLM identifies the correct answer among the top-k paragraphs retrieved by the QR-RAG system. In specialized domains like water oxidation catalysts, retrieved documents often contain significant noise due to high semantic overlap. Despite these similarities, the LLM demonstrates its ability to interpret the scientific context and evaluate specific constraints within the query. This ensures the precise identification of the actual answer among numerous similar candidates, resulting in highly reliable outputs such as accurate DOIs.



Supplementary Fig 11. Effect of database size on DOI identification Q/A accuracy using QR-RAG with structured (JSON) database and LLaMA 3.3-70B. Blue diamonds represent subsets of the OER database, the red square indicates the full OER database (2,343 papers), and the green star shows performance when the battery database (5,000 papers) is added to the full OER database.

DOI identification question list (202 questions)

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| What is the DOI of the paper that explores the use of <i>Tectona grandis</i> leaves for synthesizing carbon nanodots (CNDs) and their incorporation into a bimetallic MOF for enhanced OER activity? |
| What is the DOI of paper that investigates hollow core-shell particles where the shell component derives from terephthalic acid coordination, studies how the Kirkendall effect relates to structural development, and examines surface wettability changes after heat treatment? |
| What is the DOI of the paper connects the formation of nanostructured materials to soft-templating mechanisms, analyzes crystallinity changes using diffraction techniques, and explores how oxidation state distributions relate to electron transfer kinetics during catalysis? |
| What is the DOI of the paper that explores nitrogen and phosphorus-rich carbon frameworks with nickel phosphide for bifunctional water splitting catalysis? |
| What is the DOI of the paper that discusses melamine-assisted synthesis approach for anchoring nickel phosphide in dual-element doped carbon matrices for water splitting? |
| What is the DOI of the paper that investigates the thickness and stability of nanosheets formed through chronoamperometric treatment at different potentials and durations? |
| What is the DOI of the paper that develops a core-shell heterostructure by growing $\text{Fe}(\text{OH})_3$ on $\text{Co}(\text{OH})\text{F}/\text{Ni}(\text{OH})_2$ nanosheets through interfacial hydrolysis? |
| What is the DOI of the paper that synthesized a NiCo_2O_4 nanostructure supported on reduced graphene oxide through a controlled hydrothermal reaction protocol, exhibiting low onset potential for both HER and OER? |
| What is the DOI of the paper that studies copper-doped cobalt oxide electrodes for electrocatalytic oxidation of cyanide in alkaline media? |
| What is the DOI of the paper that studies nitrogen-doped carbon dots supported NiFe layered double hydroxide in alkaline medium? |
| What is the DOI of the paper that describes a graphene-templated growth of $\text{MoS}_2\text{-Ni}_3\text{S}_2$ heterostructures for efficient overall water splitting? |
| What is the DOI of the paper that studies the formation of oxyhydroxide catalytic active species during the OER process using Fourier-transformed alternating current voltammetry? |
| What is the DOI of the paper that studies core-shell structured nanoparticles synthesized from DMF solution with multiple metal acetates, which shows both excellent alkaline and seawater electrolysis performance? |
| What is the DOI of the paper that synthesized $\text{Fe}_{0.2}\text{NiCo}_{1.8}\text{Se}_4$ nanorod arrays on carbon cloth through a hydrothermal method using FeCl_3 , nickel chloride, cobalt chloride, and sodium selenite as precursors? |
| What is the DOI of the paper that uses silver doping to improve conductivity of metal oxides, employs hydrothermal strategy on nickel foam, and evaluates oxygen vacancy effects on catalytic performance? |
| What is the DOI of the paper that describes a strategy of replacing oxygen evolution reaction with thermodynamically favorable hydrazine oxidation reaction to avoid chlorine evolution? |
| What is the DOI of the paper that presents a strategy for tuning surface energy density of non-stoichiometric perovskite by creating surface defects through a colloidal template strategy? |
| What is the DOI of the paper that details the development of hollow cobalt-borate modified cobalt oxide catalysts derived from zeolitic imidazolate frameworks for electrocatalytic water splitting? |
| What is the DOI of the paper that explores how hexadecyltrimethylammonium hydroxide promotes electrocatalytic activity for the oxygen evolution reaction? |
| What is the DOI of the paper that fabricated tube brush-like $\text{Co}_3\text{S}_4@\text{NiCo-LDH}$ nanoarrays on Ni foam using a three-step hydrothermal method involving $\text{Co}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$, $\text{Na}_2\text{S} \cdot 9\text{H}_2\text{O}$, and $\text{Ni}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$? |
| What is the DOI of the paper that investigates how partial phosphidation creates a self-supporting MOF-nanoparticle hybrid for efficient urea oxidation and hydrogen evolution reactions? |
| What is the DOI of the paper that investigates hierarchical bimetallic phosphide structures derived from layered precursors for water oxidation? |
| What is the DOI of the paper that demonstrates how annealing temperature controls the crystallinity of cobalt borides and their transformation into catalytically active oxyhydroxides during oxygen evolution? |
| What is the DOI of the paper where $\text{NiSe}_2/\text{CeO}_2$ nanocomposites are synthesized via hydrothermal |

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| synthesis followed by solid-state thermolysis and optimized for OER at 10 mA cm ⁻² ? |
| What is the DOI of the paper that explores the use of flexible three-dimensional electrodes containing molybdenum compounds for full water splitting in acidic electrolytes and achieves an onset potential lower than -20 mV vs. RHE for HER and below +1.45 V vs. RHE for OER? |
| What is the DOI of the paper that proposes controlled charge transfer from cobalt to molybdenum carbide to manipulate electronic properties for enhanced oxygen evolution? |
| What is the DOI of the paper that investigates how cobalt incorporation transforms primarily HER-active molybdenum carbide into a bifunctional catalyst through controlled charge redistribution? |
| What is the DOI of the paper that studies metallic Ni ₃ Se ₂ films as model catalysts to figure out structural change rules during hydrogen and oxygen evolution processes? |
| What is the DOI of the paper that investigates transition metal doping in noble metal catalysts using RuCl ₃ and IrCl ₃ precursors and examines their durability through ICP-MS measurements? |
| What is the DOI of the paper that challenges conventional understanding by showing that higher charge transfer resistance in LDH-graphene hybrid catalysts correlates with improved OER performance, explaining this through hydrophilicity and inhibition of graphene stacking? |
| What is the DOI of the paper that explores how the valence state of iridium dopant (Ir ³⁺ vs Ir ⁴⁺) in NiFe-LDH affects both hydrogen and oxygen evolution reactions? |
| What is the DOI of the paper that demonstrates how trivalent iridium ions can donate more electrons to neighboring oxygen atoms than tetravalent iridium ions in layered double hydroxides, improving water dissociation and boosting HER performance? |
| What is the DOI of the paper that elucidates the chemical nature of Ni and Fe in electrocatalysts through XANES analysis, proposing a charge transfer mechanism that accounts for high catalytic activity through a specific bond type? |
| What is the DOI of the paper that challenges the long-held view about NiOOH phase activity for OER by investigating oxidation states through in situ spectroscopy, revealing a synergistic interaction between two metals mediated by an oxygen atom? |
| What is the DOI of the paper that examines partially amorphous hollow transition metal chalcogenide structures formed through nanoscale diffusion effects, revealing that the active catalyst phase transforms during operation while maintaining its morphological advantages? |
| What is the DOI of the paper that explores how asymmetric electron spin density and charge polarization in co-doped carbon can enhance OER performance when combined with a semiconducting catalyst, while also providing a protective barrier against electrolyte degradation? |
| What is the DOI of the paper that examines how a green synthesis approach without templates or surfactants can create hierarchical chalcogenide structures with both solid cores and loose shells, providing insights into the relationship between multiscale porosity and catalyst stability? |
| What is the DOI of the paper that investigates how crystallinity affects the interface between catalyst and electrolyte, demonstrating that amorphous decoration on a perovskite backbone provides superior activity through enhanced contact area compared to crystalline counterparts? |
| What is the DOI of the paper that combines the stability advantages of a layered double perovskite with the higher surface area of a transition metal hydroxide, illustrating how crystal ordering influences charge transfer and OER reaction pathways? |
| What is the DOI of the paper that develops a bifunctional catalyst through interface engineering between a metal phosphide and a layered double hydroxide, demonstrating how their electronic interaction facilitates charge transfer that benefits both hydrogen and oxygen evolution reactions? |
| What is the DOI of the paper that reveals how a heterostructure promotes the in-situ formation of active phases during both cathodic and anodic processes, maintaining nanowire architecture while surface chemistry dynamically evolves to enhance catalytic performance? |
| What is the DOI of the paper that applies a three-dimensional carbonized polyaniline fiber structure as a support matrix for Fe-Co oxide nanoparticles, where electron redistribution between metal cores and graphitized carbon mediates oxygen adsorption energy to address OER kinetics limitations? |
| What is the DOI of the paper that develops a novel anode for efficient chlorine evolution in dilute chloride solutions by controlling OER overpotential, where cobalt oxide was selected as the electrode material with iridium added as a cocatalyst to improve stability? |
| What is the DOI of the paper that explores the counterintuitive discovery that mixed-phase cobalt oxide/cobalt monoxide demonstrates superior OER catalytic activity compared to pure-phase single oxides obtained through calcination, despite conventional wisdom favoring phase purity? |

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| What is the DOI of the paper that synthesizes Co ₃ O ₄ nanoparticles via solution combustion method where fuel-to-oxidizer ratio and pH were systematically varied, revealing that uncalcined samples with fuel-lean conditions exhibit enhanced OER performance due to their higher porosity and surface area? |
| What is the DOI of the paper that constructs a nanoforest-like heterojunction through a facile substrate etching and hydrothermal process, where electrons transfer from Cu ₂ O to NiCo ₂ O ₄ at the interface, converting relatively inert Cu(I) into active Cu(II) species for enhanced water splitting? |
| What is the DOI of the paper that compares three different transition metal-based catalysts (CoMoO ₄ , CoWO ₄ , and Co ₃ (VO ₄) ₂) after modification with FeOOH, concluding that Mo exhibits stronger electronic effects and better electrical conductivity than V and W in OER catalysis? |
| What is the DOI of the paper that describes a capillary-like porous structure with a roughened surface formed by modifying CoAl LDH with amorphous FeOOH through a simple iron chloride solution treatment? |
| What is the DOI of the paper that reports a bifunctional catalyst NiFeOH/CoS _x /NF made by first electrodepositing CoS _x on nickel foam and then hydrothermally growing NiFe hydroxide nanosheets using Ni(NO ₃) ₂ ·6H ₂ O and Fe(NO ₃) ₃ ·9H ₂ O? |
| What is the DOI of the paper that compared four different phases of MnO ₂ (α-, β-, γ-, δ-) as supports for IrO ₂ catalysts for oxygen evolution? |
| What is the DOI of the paper that attributes enhanced OER activity to edge-exposed NiO nanosheets and MoO ₃ -VC interfacial synergy, supported by SEM-derived morphology and electrochemical double-layer capacitance data? |
| What is the DOI of the paper that examines how dual N/S doping in NSG tunes electronic structure and facilitates water dissociation at Ni ₂ P sites, using DFT charge analysis and Nyquist plots from EIS measurements? |
| What is the DOI of the paper that investigates Ni ₂ P nanocrystal confinement within NSG for bifunctional catalysis, validated by TEM imaging and long-term overall water splitting data in neutral pH? |
| What is the DOI of the paper that demonstrates the electronic and catalytic impact of Co ion intercalation in NiFe LDH, supported by UV-vis bandgap narrowing and volcano-type DFT binding energy trends? |
| What is the DOI of the paper that compares Co-substitution and Co-intercalation in NiFe LDH via EXAFS coordination changes and OER faradaic efficiencies, highlighting distinct structural motifs? |
| What is the DOI of the paper that constructs a hierarchical Co-Bi nanoarray via electrochemical conversion of CoS ₂ and verifies its nanostructure through SEM-TEM analysis and stability over OER chronoamperometry? |
| What is the DOI of the paper that reports multi-time-scale charge transport and mass activity in a Co-Bi nanoarray, examined through iR-compensated polarization curves and EIS-derived charge transfer resistances? |
| What is the DOI of the paper that links improved OER in Co _{0.20} Fe _{0.80} OOH to surface-active site tuning and oxygen vacancy formation, combining XPS and Tafel analysis? |
| What is the DOI of the paper that investigates the transformation of Prussian blue analogues into hollow NiFe LDH nanoboxes, validated by operando XAS and correlated with EXAFS analysis of Fe-Co dual-site OER mechanisms? |
| What is the DOI of the paper that attributes high OER activity to Fe-Co synergistic active sites in NiFe LDH nanoboxes, combining chronoamperometric durability and ECSA trends with nanoscale structural observations? |
| What is the DOI of the paper that links NiFe(20Ni)-MOF/NFF nanosheet architecture to surface oxyhydroxide formation during activation, requiring both SEM morphology and XPS post-electrolysis data? |
| What is the DOI of the paper that correlates high pseudocapacitive behavior of SnS/Ni foam with low charge transfer resistance, combining CV sweep analysis and EIS-derived R _{ct} values? |
| What is the DOI of the paper that confirms 10-hour OER stability of hydrothermally synthesized SnS/Ni foam via post-cycling redox feature retention and SEM morphology preservation? |
| What is the DOI of the paper that attributes amorphization-induced OER enhancement in CoOOH/W18O ₄₉ to structural disorder shown in Raman spectra and lowered Tafel slope values? |

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| What is the DOI of the paper that shows optimized HER/OER bifunctionality in Act-CoOOH/W18O49/NF, integrating flat-band potential shifts from Mott–Schottky and EIS data across potentials? |
| What is the DOI of the paper that simultaneously introduces nitrogen into a mesostructured carbon framework while forming in-pore metallic cobalt nanoparticles via ammonia treatment, and attributes the enhanced oxygen-evolution turnover to electronic coupling between the doped carbon and confined cobalt? |
| What is the DOI of the paper that reveals cobalt-catalysed graphitisation of a nitrogen-doped carbon host and links the evolving support ordering to rising oxygen-evolution activity compared with mesoporous Co ₃ O ₄ ? |
| What is the DOI of the paper that engineers dandelion-like NiCoP arrays grown on nanowires, showing how the radial architecture accelerates electrolyte diffusion and preserves its morphology during extended water-splitting operation? |
| What is the DOI of the paper that ascribes the bifunctional electrocatalytic activity of amorphous NiCoP to synergistic electronic interactions between Ni and Co revealed by post-operando characterisation? |
| What is the DOI of the paper that demonstrates composition-controlled Ni–Co–S–Se alloy nanocrystals acting as precatalysts, transforming in situ into mixed metal hydroxides whose activity varies with the sulfur-to-selenium ratio? |
| What is the DOI of the paper that reports a multi-fold increase in oxygen-evolution turnover when quaternary Ni–Co–S–Se nanocrystals are tuned to produce ultra-small, highly conductive oxide domains after electrochemical activation? |
| What is the DOI of the paper that builds a NiFe LDH/FeOOH heterostructure on nickel–iron foam and shows that interfacial electron transfer both promotes rapid NiOOH formation and suppresses competing chlorine oxidation in alkaline saline water? |
| What is the DOI of the paper that uses coupled Raman and XPS analyses to demonstrate that FeOOH domains electronically activate adjacent NiFe LDH layers, enabling multi-day stable hydrogen and oxygen generation from simulated seawater? |
| What is the DOI of the paper that grows a porous film of ultrathin NiFe phosphate nanotubes on nickel foam and shows that phosphate anions stabilise high-spin Ni sites for long-duration oxygen evolution? |
| What is the DOI of the paper that employs electron-paramagnetic resonance to link oxygen-vacancy-rich amorphous NiFe-Pi to accelerated redox cycling of Ni during water oxidation over hundreds of hours? |
| What is the DOI of the paper that powers overall water splitting with only a single household battery by exploiting redox buffering between a NiFe ₂ O ₄ core and a NiFe LDH shell? |
| What is the DOI of the paper that employs an ionic liquid as both solvent and carbon source to generate Ni/Ni ₃ C core–shell nanospheres through a three-stage mechanism of Ni-catalysed carbonisation and carbide shell growth? |
| What is the DOI of the paper that attributes enhanced oxygen-evolution activity to electron-rich Ni cores coupled through a conductive carbide shell, giving rise to a characteristic Gerischer impedance response? |
| What is the DOI of the paper that fabricates a NiO/NiS heterostructure and shows that the buried semiconductor junction accelerates in-situ NiOOH nucleation, outperforming individual oxide or sulfide analogues? |
| What is the DOI of the paper that combines spectroscopic and impedance analyses to reveal how mixed-anion coordination at the NiO NiS interface tunes eg-orbital occupancy and lowers charge-transfer resistance during alkaline water oxidation? |
| What is the DOI of the paper that links the semimetallic nature of the cubic polymorph of NiP ₂ to superior hydrogen- and oxygen-evolution performance inside a proton-exchange-membrane electrolyser compared with its semiconducting monoclinic counterpart? |
| What is the DOI of the paper that uses in-situ synchrotron diffraction to show the irreversible cubic-to-monoclinic transformation of NiP ₂ and discusses how the bulk phase change reshapes surface catalytic properties? |
| What is the DOI of the paper that assembles a sheet-on-sheet NiSe@NiFe-LDH heterostructure on nickel foam, where conductive NiSe electronically wires NiFe-LDH layers to outperform RuO ₂ Pt/C in overall water splitting? |

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| What is the DOI of the paper that develops a dual-function electrode composed of Co ₃ Mo particles interfaced with CoMoO ₃ sheets, showing it can outperform conventional Pt/C and RuO ₂ catalysts in alkaline full-cell electrolysis at high current? |
| What is the DOI of the paper that investigates how strong electronic interactions at the junction between Co ₃ Mo nanoparticles and a porous CoMoO ₃ matrix promote efficient hydrogen evolution by enhancing water splitting kinetics? |
| What is the DOI of the paper that constructs a vertically aligned CoMoS ₄ nanosheet layer over a sulfide-rich Ni ₃ S ₂ underlayer and demonstrates their cooperative effect on boosting oxygen evolution in alkaline solution? |
| What is the DOI of the paper that explores a hybrid catalytic platform where Ni ₃ S ₂ improves charge transport to CoMoS ₄ nanosheets, enabling low-voltage water electrolysis in both HER and OER regimes? |
| What is the DOI of the paper that fabricates partially phosphidized cobalt nanowires with internal pores and examines how their 3D morphology influences catalytic behavior in acidic and basic water splitting? |
| What is the DOI of the paper that fine-tunes the crystallinity and surface defects of NiCo ₂ O ₄ nanorods through sulfur treatment, and evaluates their bifunctional catalytic response in water splitting? |
| What is the DOI of the paper that links the presence of abundant grain boundaries and sulfur doping in spinel nanorods to improvements in charge transfer efficiency during electrolysis? |
| What is the DOI of the paper that embeds graphene-based quantum structures into nickel–cobalt phosphide nanosheets to manipulate charge flow pathways and achieve high-rate hydrogen production? |
| What is the DOI of the paper that examines the synergy between graphene quantum dots and phosphide nanosheets in enabling efficient overall water electrolysis compared to oxide or wire-type analogs? |
| What is the DOI of the paper that shows how brief ultrasonic treatment alters the structure of NiFe LDH nanosheets, introducing defects and spacing that reduce onset potential for oxygen evolution? |
| What is the DOI of the paper that associates sonochemically induced lattice distortions in NiFe hydroxides with improved kinetics and a favorable change in the rate-limiting step for OER? |
| What is the DOI of the paper that identifies low-temperature-derived Co ₃ O ₄ microspheres with fine nanostructure as superior OER catalysts due to their abundant surface cobalt sites? |
| What is the DOI of the paper that reveals how Co ₃ O ₄ nanoparticles prepared under mild heat retain small crystal sizes, which contribute to higher OER efficiency without requiring composite strategies? |
| What is the DOI of the paper that combines layered NiFe hydroxides with a hybrid support of graphdiyne and graphene, showing that this interface engineering significantly boosts alkaline OER performance? |
| What is the DOI of the paper that contrasts the catalytic behavior of NiFe-LDH on various carbon supports and finds that coupling to graphdiyne–graphene hybrids enables both fast kinetics and long-term stability? |
| What is the DOI of the paper that builds nanoneedle-like CoMoO ₄ assemblies and links their porous internal architecture to enhanced OER and supercapacitor behavior through rapid electron-ion transport? |
| What is the DOI of the paper that compares hierarchical CoMoO ₄ with other oxide catalysts and attributes its superior OER activity to the nanosheet-based needle structure and high surface exposure? |
| What is the DOI of the paper that links the bifunctional water-splitting ability of Ni–Mo nitride heterostructures to charge redistribution at the metal nitride interfaces together with fast electron transport provided by nitrogen-doped carbon nanotube scaffolds on carbon cloth? |
| What is the DOI of the paper that describes a self-supporting electrode where encapsulated Ni/MoN clusters and a three-dimensional CNT network jointly enable the same substrate to drive both hydrogen and oxygen evolution under alkaline conditions? |
| What is the DOI of the paper that attributes superior oxygen evolution kinetics of cobalt oxide on N-CNTs to ammonia-driven nitrogen incorporation plus partial lattice reduction, which together improve conductivity and promote in-situ transformation into active oxyhydroxide layers? |
| What is the DOI of the paper that contrasts NH ₃ -treated and H ₂ -treated CoO _x /NCNT catalysts, showing that surface nitrogen enhances hydrophilicity and long-term stability even though cobalt |

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| appears in a lower formal oxidation state after the ammonia step? |
| What is the DOI of the paper that designs seaweed-like $\text{Ni}_3\text{S}_2@\text{MoS}_2@\text{Ni}_3\text{Si}_2$ hybrids whose intertwined sulfide interfaces cooperate with a conductive silicide backbone to minimise charge-transfer resistance while providing abundant edge sites for both half-reactions? |
| What is the DOI of the paper that achieves simultaneous hydrogen and oxygen catalysis by in-situ growing hierarchical sulfide–silicide structures on nickel foam, thereby combining mechanical adhesion with accelerated gas release pathways? |
| What is the DOI of the paper that fabricates defect-rich Co carbonate hydroxide cores enveloped by CoSe nanosheets, and explains how their heterointerface together with a nickel-foam current collector boosts electron migration during overall water splitting? |
| What is the DOI of the paper that employs a two-step hydrothermal route to engineer oxygen-vacancy-containing $\text{CoCO}_3 \cdot 0.5\text{H}_2\text{O}@\text{CoSe}$ nanowires whose synergistic lattice strain and conductive support underpin robust bifunctional performance? |
| What is the DOI of the paper that reports an unusual trend in $\text{Co}_2\text{Fe-LDH}/\text{N-graphene}$ hybrids where increasing hydroxide loading simultaneously raises catalytic activity and charge-transfer resistance, an effect traced to hydrophilic LDH layers preventing graphene restacking? |
| What is the DOI of the paper that confirms by rotating-ring–disk studies that the most active LDH/graphene composite follows a four-electron oxygen pathway despite exhibiting higher interfacial impedance than leaner formulations? |
| What is the DOI of the paper that introduces a chemically robust bimetallic squarate MOF whose one-dimensional Ni–Fe hydroxide strips offer open channels for electrolyte diffusion while simultaneously acting as built-in catalytic sites? |
| What is the DOI of the paper that shows tuning the Ni:Fe ratio in a squarate framework optimises both structural stability and electron transport, enabling a porous MOF to rival layered double hydroxides in oxygen evolution? |
| What is the DOI of the paper that demonstrates trivalent iridium dopants donate more electron density to neighbouring oxygen in NiFe-LDH than tetravalent iridium, thus accelerating alkaline water dissociation and hydrogen desorption? |
| What is the DOI of the paper that generalises the above valence-state effect to ruthenium and platinum dopants, concluding that oxidation state selection is a critical design lever for layered hydroxide electrocatalysts? |
| What is the DOI of the paper that upcycles yeast biomass into multi-heteroatom-doped carbon hosting both ruthenium single atoms and nanoparticles, enabling sustained solar-driven water splitting through coupled $\text{Fe}^{2+}/\text{Fe}^{4+}$ redox chemistry at the anode? |
| What is the DOI of the paper that attributes the low interfacial resistance of an $\text{Fe}_3\text{O}_4@\text{carbon}$ anode to synergistic interactions with a doped-carbon matrix, resulting in stable outdoor operation without noble-metal oxides? |
| What is the DOI of the paper that constructs sub-microwires comprising a metallic MoO_2 core clad with MoS_2 nanosheets and Ni_2P nanoparticles, so that nested electron pathways and multi-interface coupling deliver bifunctional catalysis? |
| What is the DOI of the paper that explains how temperature-programmed sulfuration followed by phosphidation transforms nickel molybdate into a tri-component hybrid whose individual phases collectively address conductivity, active-site density and reaction kinetics? |
| What is the DOI of the paper that investigates how Fe incorporation into NiS_2 affects the metallic nature and suppresses thick passivation layer formation during OER cycles? |
| What is the DOI of the paper that examines the role of Fe–S bond shortening in improving the structural resilience of NiS_2 -based electrocatalysts under alkaline OER conditions? |
| What is the DOI of the paper that utilizes molten KSCN salt and surface corrosion to fabricate amorphous-crystalline hybrid NiFe sulfide catalysts for high current density OER? |
| What is the DOI of the paper that explores the synergistic interplay between nanoglass-structured FeNi_2S_4 and amorphous NiFe–LDH in sustaining industrial-grade OER at elevated temperature and electrolyte strength? |
| What is the DOI of the paper that designs ternary $\text{CoP}_{2x}\text{Se}_2(1-x)$ nanowires through dual doping to improve water splitting performance in a single alkaline cell? |
| What is the DOI of the paper that reports how fine-tuned P-to-Se substitution in cobalt-based ternary nanowires affects HER and OER activities symmetrically in dual-electrode configurations? |

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| What is the DOI of the paper that employs etching followed by phosphorus doping to produce Fe-modified CoP nanowires optimized for dual HER and OER performance? |
| What is the DOI of the paper that correlates the optimal Fe doping ratio in Co-based phosphide nanowires with minimized overpotential in both cathodic and anodic reactions? |
| What is the DOI of the paper that demonstrates the stabilization of hollow CoP/MnO nanofibers through controlled phosphidation of MnCo_2O_4 intermediates for OER durability? |
| What is the DOI of the paper that attributes enhanced OER activity to the internal structure of CoP/MnO nanofibers designed for extended cycling stability? |
| What is the DOI of the paper that introduces fluorine as a dopant to generate oxygen vacancies and modify the band structure of cobalt molybdate nanosheets for OER catalysis? |
| What is the DOI of the paper that shows how F-induced vacancy engineering and Mo 4d orbital tuning synergistically boost OER kinetics in CoMoO_4 ? |
| What is the DOI of the paper that constructs a 3D Ni_2P - MoS_2 heterostructure on carbon cloth using a two-step conversion process to optimize bifunctional catalytic activity? |
| What is the DOI of the paper that attributes exceptional HER and OER performance to interface effects in vertically grown Ni_2P - MoS_2 nanosheet arrays? |
| What is the DOI of the paper that designs okra-shaped Cu-doped CoP/ Co_3O_4 hollow nanotube arrays and evaluates their full-cell water splitting efficiency? |
| What is the DOI of the paper that explores the dual role of vanadium in simultaneously reducing Pt clusters and enhancing charge transfer in NiFe LDH for water splitting? |
| What is the DOI of the paper that analyzes how vanadium shifts Ni's d-band center to balance adsorption-desorption energetics during OER and HER in a bifunctional electrocatalyst? |
| What is the DOI of the paper that discusses how nickel incorporation transforms FeS_2 into a semimetal with improved water affinity for oxygen evolution catalysis? |
| What is the DOI of the paper that evaluates a yolk-shell Fe-based electrocatalyst undergoing structural reformation into NiFeOOH during alkaline oxygen evolution? |
| What is the DOI of the paper that investigates the impact of gold nanoparticles on promoting NiFe layered hydroxide arrays for high-current OER in alkaline base? |
| What is the DOI of the paper that links the enhanced oxygen evolution activity of a NiFe LDH electrode to the formation of Ni^{3+} species induced by gold decoration? |
| What is the DOI of the paper that correlates superexchange interactions in Ni-Fe hydroxides with their boosted oxygen evolution efficiency in alkaline solution? |
| What is the DOI of the paper that explains the superior electrocatalytic performance of a NiFe layered hydroxide with 1.5 Ni/Fe ratio via magnetic and DEMS analysis? |
| What is the DOI of the paper that attributes enhanced oxygen evolution kinetics to a 3D-printed stainless-steel cone array coated with NiCo_2S_4 nanoneedles? |
| What is the DOI of the paper that demonstrates how structural design of metal support enables 21-fold improvement in electroactive area for water splitting? |
| What is the DOI of the paper that analyzes how high-valent cobalt doping in Fe-Ni hydroxides alters the electronic structure and enhances OER kinetics? |
| What is the DOI of the paper that evaluates a nanoneedle-based Fe-Ni-Co hydroxide electrode integrated with FeSe_2/C for supercapacitor and oxygen evolution? |
| What is the DOI of the paper that develops hierarchical NiFeV hydroxide nanotubes with V-induced charge redistribution for improved oxygen evolution performance? |
| What is the DOI of the paper that converts NiFeV hydroxide into phosphide while preserving its nanotube morphology for enhanced alkaline OER? |
| What is the DOI of the paper that reports a ternary aerogel electrode where charge separation is facilitated by codoped graphene, enabling both HER and OER under basic conditions? |
| What is the DOI of the paper that details an in situ hybrid of WSe_2 and NiFe-LDH assembled on N,S-rGO framework using a hydrothermal method for bifunctional energy devices? |
| What is the DOI of the paper that discusses HER and UOR activity enhancement through tailoring Co/Mo ratios in vertically grown sulfide nanosheets? |
| What is the DOI of the paper that explores how Mo incorporation into CoS_2 reshapes surface morphology and boosts alkaline electrocatalysis? |
| What is the DOI of the paper that investigates OER performance improvement through direct integration of a trimetallic hydroxide cluster onto Ti_3C_2 MXene? |

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| What is the DOI of the paper that attributes enhanced oxygen evolution activity to increased electron density near the Fermi level via metal–MXene interaction? |
| What is the DOI of the paper that shows SAC performance maximization by tuning Ni/Fe mass ratio below a critical threshold during carbon-supported catalyst formation? |
| What is the DOI of the paper that presents carbon-supported NiFe single-atom catalysts fabricated via one-step pyrolysis and optimized for low-resistance OER? |
| What is the DOI of the paper that leverages composition-gradient NiFe hydroxides to engineer continuous electron pathways and boost OER activity? |
| What is the DOI of the paper that describes a hydrothermal synthesis where trisodium citrate promotes gradient nanosheet formation on Ni foam for electrocatalysis? |
| What is the DOI of the paper that introduces a one-pot embedding of Pt nanoparticles into Ni–Fe Prussian blue analog nanocubes for bifunctional water splitting? |
| What is the DOI of the paper that reports a porous nanocube electrocatalyst where acid etching enhances surface area for both HER and OER? |
| What is the DOI of the paper that develops a self-supported bifunctional electrode via phosphidation of oxidized cobalt foil for water splitting? |
| What is the DOI of the paper that identifies P-top sites in Co ₂ P as active centers for HER using both experimental and DFT analyses? |
| What is the DOI of the paper that fabricates TiO ₂ -based electrocatalysts where surface Zn dissolution triggers a self-optimizing structure for chlorate production? |
| What is the DOI of the paper that enhances CER selectivity via co-deposition and post-treatment of Zn–Ru–Ti alloys leading to a rough, porous TiO ₂ matrix? |
| What is the DOI of the paper that constructs ~50 nm hollow nanospheres of nickel oxysulfide through solvothermal growth for bifunctional electrocatalysis? |
| What is the DOI of the paper that assesses HER/OER activity of fullerene-mimetic Ni-based nanospheres supported on nickel foam? |
| What is the DOI of the paper that fabricates FCC-Ni/NiS heterostructures within N,S-doped rGO via stepwise annealing of coordination polymer/GO hybrids? |
| What is the DOI of the paper that attributes enhanced OER activity to multiphase interfaces and nanoscale layering in a hybrid Ni-based composite? |
| What is the DOI of the paper that demonstrates how incorporating a fourth transition metal improves the reaction rate at high current densities in a FeCoNi-based alloy? |
| What is the DOI of the paper that achieves phosphide formation without using hazardous phosphorus donors by transforming LDH nanosheets in hydrogen atmosphere? |
| What is the DOI of the paper that relates electrocatalytic activity to spin configuration and electron redistribution at Ni-based active centers? |
| What is the DOI of the paper that shows OER efficiency peaks at specific d-band values when doping Ni-MOFs with various 3d metals? |
| What is the DOI of the paper that constructs hollow tri-metal selenide nanostructures by leveraging template-directed carbon frameworks? |
| What is the DOI of the paper that achieves dual electrocatalysis by integrating Cu, Ni, and Co into selenide nanosheets supported on nitrogen-rich scaffolds? |
| What is the DOI of the paper that identifies 200 °C as the optimal condition for achieving low overpotential in Mo-doped Ni ₃ S ₂ grown on conductive substrates? |
| What is the DOI of the paper that attributes OER activity enhancement to thermally induced oxygen vacancy formation in nanobelt catalysts? |
| What is the DOI of the paper that tunes oxygen vacancy levels in spinel-type nanobelts through inert atmosphere annealing at different temperatures? |
| What is the DOI of the paper that explains OER enhancement through synergistic interplay in a nickel oxide–phosphide core–shell nanosheet architecture? |
| What is the DOI of the paper that synthesizes hollow Co–Fe phosphide microtubes through multistep conversion from metal–organic precursors? |
| What is the DOI of the paper that applies a urea–based method to produce conductive hafnium nitride nanoparticles for oxygen electrocatalysis? |
| What is the DOI of the paper that emphasizes long-term catalyst durability in alkaline OER using a metal nitride not previously tested? |

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| What is the DOI of the paper that constructs high-performing anodes by directly converting Ni foam with iron and vanadium ions without using deposition techniques? |
| What is the DOI of the paper that investigates seawater electrolysis using a hierarchical IrO ₂ @MnO ₂ structure supported by reduced graphene oxide? |
| What is the DOI of the paper that evaluates FeNi ₃ @Ni nanoparticles for durability in AMF-enhanced electrolysis via ILTEM and in situ XRD? |
| What is the DOI of the paper that explores the long-term crystallographic transformations of FeNi ₃ @Ni under reductive and oxidative conditions up to 600°C? |
| What is the DOI of the paper that attributes enhanced OER activity to a synergistic interface between FeOOH and hollow NiCoP/C nanocages? |
| What is the DOI of the paper that demonstrates electron redistribution at a coupling interface between FeOOH and NiCoP/C improves OER intermediate adsorption? |
| What is the DOI of the paper that achieves dual HER and OER activity using porous nitrogen-doped carbon nanofibers embedded with cobalt nanoparticles? |
| What is the DOI of the paper that uses an electrospinning method followed by acid etching to create porous Co-PNCNFs with high OER current density? |
| What is the DOI of the paper that develops amorphous iron oxide nanosheet arrays via electrochemical desulfurization for self-supported OER electrodes? |
| What is the DOI of the paper that reports enhanced OER activity after long-term operation of FeOx nanosheets grown on carbon cloth? |
| What is the DOI of the paper that enhances Ni(OH) ₂ OER performance by pillaring it with zero-dimensional polyoxovanadate clusters? |
| What is the DOI of the paper that forms a 2D/0D nanohybrid of Ni(OH) ₂ and polyoxovanadates via chemical solution growth in decarbonated water? |
| What is the DOI of the paper that synthesizes Fe ₂ Co ₈ HCF nanospheres with a core-shell structure showing bifunctional water splitting activity at 1.63 V? |
| What is the DOI of the paper that attributes high OER and HER performance to interfacial strain and electronic redistribution in Fe ₂ Co ₈ HCF core-shell catalysts? |
| What is the DOI of the paper that investigates how increasing Co ₂ Fe LDH loading on N-doped graphene paradoxically raises charge transfer resistance while enhancing OER activity? |
| What is the DOI of the paper that attributes improved OER performance of Co ₂ Fe LDH–N-graphene hybrids to inhibition of graphene stacking and uniform LDH dispersion? |
| What is the DOI of the paper that constructs a three-dimensionally stretched film by in-situ polymerizing sodium anthraquinone-2-sulfonate on hydrothermally grown Ni ₃ S ₂ nanosheets and attributes its bifunctional electrocatalytic activity to synergistic quinone–sulfide interactions revealed by operando Raman and DFT analysis? |
| What is the DOI of the study that reports an ultrathin anthraquinone polymer film draped over Ni ₃ S ₂ nanosheets forming a “3D-stretched” architecture whose long-term alkaline durability is linked to interfacial π–d conjugation between the polymer and metal sulfide? |
| What is the DOI of the article that engineers defect-rich NiO sheaths around NiMoO ₄ nanorods, enabling a three-stage Fe capture process adsorption, migration, and impregnation that reconstructs the surface into active oxyhydroxide layers during water oxidation? |
| What is the DOI of the study that links the persistent Co ²⁺ /Co ³⁺ redox couple and low charge-transfer resistance of a CoS/CNT nanocomposite to intimate sulfide–carbon contacts verified by X-ray photoelectron spectroscopy and chronoamperometry cycling? |

Supplementary Table 1. DOI identification questions for OER quantitative evaluation (n=202). All questions are formulated to request the DOI based on one or more specific conditions.

Numerical property extraction question list (50 questions)

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| In the hydrothermal synthesis of $\text{CoMoO}_4 \cdot \text{H}_2\text{O}$ with a reaction time of 6 hours, what is the reaction temperature? |
| What is the overpotential of M-C@CFOSs to reach 10 mA cm^{-2} for OER? |
| What is the overpotential of HNP to reach 10 mA cm^{-2} for OER? |
| What is the Tafel slope of LFNSe-III for the oxygen evolution reaction? |
| In the hydrothermal synthesis of NiOF using nickel(II) chloride hexahydrate as precursor with a reaction time of 1 hours under air atmosphere, what is the reaction temperature? |
| In the hydrothermal synthesis of DS--NiFe LDH using $\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$ as precursor with a reaction time of 8 hours under nitrogen atmosphere, what is the reaction temperature? |
| What is the Tafel slope of NiCo/Ni/CuO/CF for the oxygen evolution reaction? |
| What is the Tafel slope of K-ZIF-67-Ac-800 for the oxygen evolution reaction? |
| What is the Tafel slope of CoOx/FeOx/CNTs for the oxygen evolution reaction? |
| In the hydrothermal synthesis of CuCo_2Se_4 with a reaction time of 24 hours, what is the reaction temperature? |
| In the hydrothermal synthesis of CoFe-BDC using $\text{Co}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ as precursor with a reaction time of 12 hours, what is the reaction temperature? |
| What is the Tafel slope of CC@CoO@FeOOH-NWAs for the oxygen evolution reaction? |
| In the hydrothermal synthesis of $\text{CoFeZr}_{0.1}/\text{NCBC}$ using $\text{FeCl}_3 \cdot 6\text{H}_2\text{O}$ as precursor with a reaction time of 15 hours, what is the reaction temperature? |
| What is the Tafel slope of C@NiCo ₁₂ for the oxygen evolution reaction? |
| What is the Tafel slope of RuNiOx for the oxygen evolution reaction? |
| In the hydrothermal synthesis of Mo-Co ₉ Se ₈ @NiSe/NF using SeO_2 as precursor with a reaction time of 8 hours, what is the reaction temperature? |
| In the hydrothermal synthesis of $\text{Co}_3\text{O}_4/\text{NF}$ with a reaction time of 6 hours, what is the reaction temperature? |
| What is the Tafel slope of V-Ni ₃ N/NF for OER in 1 M KOH? |
| In the hydrothermal synthesis of Framework using $\text{Co}(\text{SO}_4) \cdot 6\text{H}_2\text{O}$ as precursor with a reaction time of 2 hours, what is the reaction temperature? |
| What is the Tafel slope of ZIF@Ni-B-Co for the oxygen evolution reaction? |
| In the hydrothermal synthesis of Co/P-N-C with a reaction time of 10 hours, what is the reaction temperature? |
| What is the Tafel slope of NiFe-UMNs for the oxygen evolution reaction? |
| What is the overpotential of Ni ₄ Mo/MoO ₂ /C-10 to reach 10 mA cm^{-2} for OER? |
| What is the overpotential of Mo-Ni ₂ P/NF to reach 40 mA cm^{-2} for OER? |
| What is the Tafel slope of Zr ₅₀₀ -MSNF for the oxygen evolution reaction? |
| What is the Tafel slope of Co ₉ S ₈ -SWCNT for the oxygen evolution reaction? |
| In the hydrothermal synthesis of Fe-Co-P catalyst using iron chloride as precursor with a reaction time of 12 hours, what is the reaction temperature? |
| What is the Tafel slope of BSCF-12 for OER in 1 M KOH? |
| What is the overpotential of Fe ₂ O ₃ @h-Co ₉ S ₈ @C to reach 10 mA cm^{-2} for OER? |
| What is the Tafel slope of MnFe ₂ O ₄ /BC for OER in 1 m KOH? |
| What is the overpotential of Ni ₉ Fe ₁ to reach 100 mA cm^{-2} for OER? |
| What is the overpotential of NiFeS/CoS to reach 150 mA cm^{-2} for OER? |
| What is the Tafel slope of Fe ₂ Co ₈ HCF for the oxygen evolution reaction? |
| What is the Tafel slope of Co-Cu(BDC)/GC for the oxygen evolution reaction? |
| In the hydrothermal synthesis of NaOH with a reaction time of 4 hours, what is the reaction temperature? |
| What is the Tafel slope of WO ₃ /Ni for the oxygen evolution reaction? |

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| In the hydrothermal synthesis of MoS ₂ /CoB/CC using CoCl ₂ ·6H ₂ O as precursor, what is the reaction temperature? |
| In the hydrothermal synthesis of OGFs with a reaction time of 12 hours, what is the reaction temperature? |
| What is the Tafel slope of IrO _x @Ni/Co-ZIF-67 for the oxygen evolution reaction? |
| In the hydrothermal synthesis of CoFe ₂ O ₄ @NF with a reaction time of 7 hours, what is the reaction temperature? |
| What is the Tafel slope of Ni/Co-DH-2 for OER in 1 M KOH? |
| In the hydrothermal synthesis of CoO-BP-RGO with a reaction time of 1 hours, what is the reaction temperature? |
| In the hydrothermal synthesis of PdO@Co ₃ O ₄ with a reaction time of 12 hours, what is the reaction temperature? |
| What is the overpotential of Co-MOF/Fe ₁₀ to reach 10 mA cm ⁻² for OER? |
| In the hydrothermal synthesis of NiCoP with a reaction time of 10 hours, what is the reaction temperature? |
| In the hydrothermal synthesis of SnO ₂ -Sb(13 - x)-Ru(x)-Pt(3) using SnCl ₄ ·5H ₂ O as precursor with a reaction time of 1 hours, what is the reaction temperature? |
| In the hydrothermal synthesis of CoSe ₂ @MoSe ₂ hollow heterostructures using CoSe ₂ hollow nanocubes as precursor with a reaction time of 15 hours, what is the reaction temperature? |
| What is the Tafel slope of NiFe/Co ₉ S ₈ /CC for the oxygen evolution reaction? |
| In the hydrothermal synthesis of NiCo-LDH@HOS with a reaction time of 4 hours, what is the reaction temperature? |
| What is the Tafel slope of S ₂ CoCd-350 for the oxygen evolution reaction? |

Supplementary Table 2. Numerical property extraction questions for OER quantitative evaluation (n=50).

All questions are formulated to request specific values including synthesis temperature, overpotential, and Tafel slope.

| Descriptive question list (202 questions) |
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| What evidence does the paper that explores the use of Tectona grandis leaves for synthesizing carbon nanodots (CNDs) and their incorporation into a bimetallic MOF for enhanced OER activity present? |
| How does the paper that investigates hollow core-shell particles where the shell component derives from terephthalic acid coordination, studies how the Kirkendall effect relates to structural development, and examines surface wettability changes after heat treatment explain its findings? |
| Which data connect the observations in the paper that connects the formation of nanostructured materials to soft-templating mechanisms, analyzes crystallinity changes using diffraction techniques, and explores how oxidation state distributions relate to electron transfer kinetics during catalysis support this connection? |
| What evidence does the paper that explores nitrogen and phosphorus-rich carbon frameworks with nickel phosphide for bifunctional water splitting catalysis present? |
| What mechanistic explanation does the paper that discusses melamine-assisted synthesis approach for anchoring nickel phosphide in dual-element doped carbon matrices for water splitting provide? |
| How does the paper that investigates the thickness and stability of nanosheets formed through chronoamperometric treatment at different potentials and durations explain its findings? |
| How does the paper that develops a core-shell heterostructure by growing Fe(OH) ₃ on Co(OH)F/Ni(OH) ₂ nanosheets through interfacial hydrolysis relate its architecture to electrocatalytic behavior? |
| Why does the paper that synthesized a NiCo ₂ O ₄ nanostructure supported on reduced graphene oxide through a controlled hydrothermal reaction protocol, exhibiting low onset potential for both HER and OER attribute such low potentials to its material design? |
| How does the paper that studies copper-doped cobalt oxide electrodes for electrocatalytic oxidation of cyanide in alkaline media explain the observed catalytic enhancement? |
| How does the paper that studies nitrogen-doped carbon dots supported NiFe layered double hydroxide in alkaline medium explain the observed catalytic enhancement? |
| Which synergistic effects are detailed in the paper that describes a graphene-templated growth of MoS ₂ -Ni ₃ S ₂ heterostructures for efficient overall water splitting? |
| How does the paper that studies the formation of oxyhydroxide catalytic active species during the OER process using Fourier-transformed alternating current voltammetry explain the observed catalytic enhancement? |
| How does the paper that studies core-shell structured nanoparticles synthesized from DMF solution with multiple metal acetates, which shows both excellent alkaline and seawater electrolysis performance explain the observed catalytic enhancement? |
| Why does the paper that synthesized Fe _{0.2} NiCo _{1.8} Se ₄ nanorod arrays on carbon cloth through a hydrothermal method using FeCl ₃ , nickel chloride, cobalt chloride, and sodium selenite as precursors attribute such low potentials to its material design? |
| How does the paper that uses silver doping to improve conductivity of metal oxides, employs hydrothermal strategy on nickel foam, and evaluates oxygen vacancy effects on catalytic performance explain its findings? |
| Which synergistic effects are detailed in the paper that describes a strategy of replacing oxygen evolution reaction with thermodynamically favorable hydrazine oxidation reaction to avoid chlorine evolution? |
| How does the paper that presents a strategy for tuning surface energy density of non-stoichiometric perovskite by creating surface defects through a colloidal template strategy explain its findings? |
| How does the paper that details the development of hollow cobalt-borate modified cobalt oxide catalysts derived from zeolitic imidazolate frameworks for electrocatalytic water splitting explain its findings? |
| What evidence does the paper that explores how hexadecyltrimethylammonium hydroxide promotes electrocatalytic activity for the oxygen evolution reaction present? |
| How does the paper that fabricated tube brush-like Co ₃ S ₄ @NiCo-LDH nanoarrays on Ni foam using a three-step hydrothermal method involving Co(NO ₃) ₂ ·6H ₂ O, Na ₂ S·9H ₂ O, and Ni(NO ₃) ₂ ·6H ₂ O explain its findings? |
| How does the paper that investigates how partial phosphidation creates a self-supporting MOF-nanoparticle hybrid for efficient urea oxidation and hydrogen evolution reactions explain its findings? |
| How does the paper that investigates hierarchical bimetallic phosphide structures derived from layered precursors for water oxidation explain its findings? |

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| How does the paper that demonstrates how annealing temperature controls the crystallinity of cobalt borides and their transformation into catalytically active oxyhydroxides during oxygen evolution explain its findings? |
| How does the paper that where NiSe ₂ /CeO ₂ nanocomposites are synthesized via hydrothermal synthesis followed by solid-state thermolysis and optimized for OER at 10 mA cm ⁻² explain its findings? |
| What evidence does the paper that explores the use of flexible three-dimensional electrodes containing molybdenum compounds for full water splitting in acidic electrolytes and achieves an onset potential lower than -20 mV vs. RHE for HER and below +1.45 V vs. RHE for OER present? |
| What mechanism is proposed in the paper that proposes controlled charge transfer from cobalt to molybdenum carbide to manipulate electronic properties for enhanced oxygen evolution ? |
| How does the paper that investigates how cobalt incorporation transforms primarily HER-active molybdenum carbide into a bifunctional catalyst through controlled charge redistribution explain its findings? |
| How does the paper that studies metallic Ni ₃ Se ₂ films as model catalysts to figure out structural change rules during hydrogen and oxygen evolution processes explain the observed catalytic enhancement? |
| How does the paper that investigates transition metal doping in noble metal catalysts using RuCl ₃ and IrCl ₃ precursors and examines their durability through ICP-MS measurements explain its findings? |
| How does the paper that challenges conventional understanding by showing that higher charge transfer resistance in LDH-graphene hybrid catalysts correlates with improved OER performance, explaining this through hydrophilicity and inhibition of graphene stacking explain its findings? |
| What evidence does the paper that explores how the valence state of iridium dopant (Ir ³⁺ vs Ir ⁴⁺) in NiFe-LDH affects both hydrogen and oxygen evolution reactions present? |
| How does the paper that demonstrates how trivalent iridium ions can donate more electrons to neighboring oxygen atoms than tetravalent iridium ions in layered double hydroxides, improving water dissociation and boosting HER performance explain its findings? |
| How does the paper that elucidates the chemical nature of Ni and Fe in electrocatalysts through XANES analysis, proposing a charge transfer mechanism that accounts for high catalytic activity through a specific bond type explain its findings? |
| How does the paper that challenges the long-held view about NiOOH phase activity for OER by investigating oxidation states through in situ spectroscopy, revealing a synergistic interaction between two metals mediated by an oxygen atom explain its findings? |
| What evidence does the paper that examines partially amorphous hollow transition metal chalcogenide structures formed through nanoscale diffusion effects, revealing that the active catalyst phase transforms during operation while maintaining its morphological advantages present? |
| What evidence does the paper that explores how asymmetric electron spin density and charge polarization in co-doped carbon can enhance OER performance when combined with a semiconducting catalyst, while also providing a protective barrier against electrolyte degradation present? |
| What evidence does the paper that examines how a green synthesis approach without templates or surfactants can create hierarchical chalcogenide structures with both solid cores and loose shells, providing insights into the relationship between multiscale porosity and catalyst stability present? |
| How does the paper that investigates how crystallinity affects the interface between catalyst and electrolyte, demonstrating that amorphous decoration on a perovskite backbone provides superior activity through enhanced contact area compared to crystalline counterparts explain its findings? |
| How does the paper that combines the stability advantages of a layered double perovskite with the higher surface area of a transition metal hydroxide, illustrating how crystal ordering influences charge transfer and OER reaction pathways explain its findings? |
| How does the paper that develops a bifunctional catalyst through interface engineering between a metal phosphide and a layered double hydroxide, demonstrating how their electronic interaction facilitates charge transfer that benefits both hydrogen and oxygen evolution reactions relate its architecture to electrocatalytic behavior? |
| How does the paper that reveals how a heterostructure promotes the in-situ formation of active phases during both cathodic and anodic processes, maintaining nanowire architecture while surface chemistry dynamically evolves to enhance catalytic performance explain its findings? |
| How does the paper that applies a three-dimensional carbonized polyaniline fiber structure as a support matrix for Fe-Co oxide nanoparticles, where electron redistribution between metal cores and graphitized carbon mediates oxygen adsorption energy to address OER kinetics limitations explain its findings? |

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| How does the paper that develops a novel anode for efficient chlorine evolution in dilute chloride solutions by controlling OER overpotential, where cobalt oxide was selected as the electrode material with iridium added as a cocatalyst to improve stability relate its architecture to electrocatalytic behavior? |
| What evidence does the paper that explores the counterintuitive discovery that mixed-phase cobalt oxide/cobalt monoxide demonstrates superior OER catalytic activity compared to pure-phase single oxides obtained through calcination, despite conventional wisdom favoring phase purity present? |
| How does the paper that synthesizes Co ₃ O ₄ nanoparticles via solution combustion method where fuel-to-oxidizer ratio and pH were systematically varied, revealing that uncalcined samples with fuel-lean conditions exhibit enhanced OER performance due to their higher porosity and surface area explain its findings? |
| How does the paper that constructs a nanoforest-like heterojunction through a facile substrate etching and hydrothermal process, where electrons transfer from Cu ₂ O to NiCo ₂ O ₄ at the interface, converting relatively inert Cu(I) into active Cu(II) species for enhanced water splitting explain its findings? |
| How does the paper that compares three different transition metal-based catalysts (CoMoO ₄ , CoWO ₄ , and Co ₃ (VO ₄) ₂) after modification with FeOOH, concluding that Mo exhibits stronger electronic effects and better electrical conductivity than V and W in OER catalysis explain its findings? |
| Which synergistic effects are detailed in the paper that describes a capillary-like porous structure with a roughened surface formed by modifying CoAl LDH with amorphous FeOOH through a simple iron chloride solution treatment? |
| How does the paper that reports a bifunctional catalyst NiFeOH/CoS _x /NF made by first electrodepositing CoS _x on nickel foam and then hydrothermally growing NiFe hydroxide nanosheets using Ni(NO ₃) ₂ ·6H ₂ O and Fe(NO ₃) ₃ ·9H ₂ O explain its findings? |
| How does the paper that compared four different phases of MnO ₂ (α-, β-, γ-, δ-) as supports for IrO ₂ catalysts for oxygen evolution explain its findings? |
| How does the paper that attributes enhanced OER activity to edge-exposed NiO nanosheets and MoO ₃ -VC interfacial synergy, supported by SEM-derived morphology and electrochemical double-layer capacitance data explain its findings? |
| What evidence does the paper that examines how dual N/S doping in NSG tunes electronic structure and facilitates water dissociation at Ni ₂ P sites, using DFT charge analysis and Nyquist plots from EIS measurements present? |
| How does the paper that investigates Ni ₂ P nanocrystal confinement within NSG for bifunctional catalysis, validated by TEM imaging and long-term overall water splitting data in neutral pH explain its findings? |
| How does the paper that demonstrates the electronic and catalytic impact of Co ion intercalation in NiFe LDH, supported by UV-vis bandgap narrowing and volcano-type DFT binding energy trends explain its findings? |
| How does the paper that compares Co-substitution and Co-intercalation in NiFe LDH via EXAFS coordination changes and OER faradaic efficiencies, highlighting distinct structural motifs explain its findings? |
| How does the paper that constructs a hierarchical Co-Bi nanoarray via electrochemical conversion of CoS ₂ and verifies its nanostructure through SEM-TEM analysis and stability over OER chronoamperometry explain its findings? |
| How does the paper that reports multi-time-scale charge transport and mass activity in a Co-Bi nanoarray, examined through iR-compensated polarization curves and EIS-derived charge transfer resistances explain its findings? |
| How does the paper that links improved OER in Co _{0.20} Fe _{0.80} OOH to surface-active site tuning and oxygen vacancy formation, combining XPS and Tafel analysis explain its findings? |
| How does the paper that investigates the transformation of Prussian blue analogues into hollow NiFe LDH nanoboxes, validated by operando XAS and correlated with EXAFS analysis of Fe-Co dual-site OER mechanisms explain its findings? |
| How does the paper that attributes high OER activity to Fe-Co synergistic active sites in NiFe LDH nanoboxes, combining chronoamperometric durability and ECSA trends with nanoscale structural observations explain its findings? |
| How does the paper that links NiFe(20Ni)-MOF/NFF nanosheet architecture to surface oxyhydroxide formation during activation, requiring both SEM morphology and XPS post-electrolysis data explain its findings? |
| How does the paper that correlates high pseudocapacitive behavior of SnS/Ni foam with low charge transfer resistance, combining CV sweep analysis and EIS-derived R _{ct} values explain its findings? |
| How does the paper that confirms 10-hour OER stability of hydrothermally synthesized SnS/Ni foam |

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| via post-cycling redox feature retention and SEM morphology preservation explain its findings? |
| How does the paper that attributes amorphization-induced OER enhancement in CoOOH/W18O49 to structural disorder shown in Raman spectra and lowered Tafel slope values explain its findings? |
| How does the paper that shows optimized HER/OER bifunctionality in Act-CoOOH/W18O49/NF, integrating flat-band potential shifts from Mott–Schottky and EIS data across potentials explain its findings? |
| How does the paper that simultaneously introduces nitrogen into a mesostructured carbon framework while forming in-pore metallic cobalt nanoparticles via ammonia treatment, and attributes the enhanced oxygen-evolution turnover to electronic coupling between the doped carbon and confined cobalt explain its findings? |
| How does the paper that reveals cobalt-catalysed graphitisation of a nitrogen-doped carbon host and links the evolving support ordering to rising oxygen-evolution activity compared with mesoporous Co ₃ O ₄ explain its findings? |
| How does the paper that engineers dandelion-like NiCoP arrays grown on nanowires, showing how the radial architecture accelerates electrolyte diffusion and preserves its morphology during extended water-splitting operation explain its findings? |
| How does the paper that ascribes the bifunctional electrocatalytic activity of amorphous NiCoP to synergistic electronic interactions between Ni and Co revealed by post-operando characterisation explain its findings? |
| How does the paper that demonstrates composition-controlled Ni–Co–S–Se alloy nanocrystals acting as precatalysts, transforming in situ into mixed metal hydroxides whose activity varies with the sulfur-to-selenium ratio explain its findings? |
| How does the paper that reports a multi-fold increase in oxygen-evolution turnover when quaternary Ni–Co–S–Se nanocrystals are tuned to produce ultra-small, highly conductive oxide domains after electrochemical activation explain its findings? |
| How does the paper that builds a NiFe LDH/FeOOH heterostructure on nickel–iron foam and shows that interfacial electron transfer both promotes rapid NiOOH formation and suppresses competing chlorine oxidation in alkaline saline water explain its findings? |
| How does the paper that uses coupled Raman and XPS analyses to demonstrate that FeOOH domains electronically activate adjacent NiFe LDH layers, enabling multi-day stable hydrogen and oxygen generation from simulated seawater explain its findings? |
| How does the paper that grows a porous film of ultrathin NiFe phosphate nanotubes on nickel foam and shows that phosphate anions stabilise high-spin Ni sites for long-duration oxygen evolution explain its findings? |
| How does the paper that employs electron-paramagnetic resonance to link oxygen-vacancy-rich amorphous NiFe-Pi to accelerated redox cycling of Ni during water oxidation over hundreds of hours explain its findings? |
| How does the paper that powers overall water splitting with only a single household battery by exploiting redox buffering between a NiFe ₂ O ₄ core and a NiFe LDH shell explain its findings? |
| How does the paper that employs an ionic liquid as both solvent and carbon source to generate Ni/Ni ₃ C core–shell nanospheres through a three-stage mechanism of Ni-catalysed carbonisation and carbide shell growth explain its findings? |
| How does the paper that attributes enhanced oxygen-evolution activity to electron-rich Ni cores coupled through a conductive carbide shell, giving rise to a characteristic Gerischer impedance response explain its findings? |
| How does the paper that fabricates a NiO/NiS heterostructure and shows that the buried semiconductor junction accelerates in-situ NiOOH nucleation, outperforming individual oxide or sulfide analogues explain its findings? |
| How does the paper that combines spectroscopic and impedance analyses to reveal how mixed-anion coordination at the NiO NiS interface tunes eg-orbital occupancy and lowers charge-transfer resistance during alkaline water oxidation explain its findings? |
| How does the paper that links the semimetallic nature of the cubic polymorph of NiP ₂ to superior hydrogen- and oxygen-evolution performance inside a proton-exchange-membrane electrolyser compared with its semiconducting monoclinic counterpart explain its findings? |
| How does the paper that uses in-situ synchrotron diffraction to show the irreversible cubic-to-monoclinic transformation of NiP ₂ and discusses how the bulk phase change reshapes surface catalytic properties explain its findings? |
| How does the paper that assembles a sheet-on-sheet NiSe@NiFe-LDH heterostructure on nickel foam, where conductive NiSe electronically wires NiFe-LDH layers to outperform RuO ₂ Pt/C in overall water splitting explain its findings? |

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| How does the paper that develops a dual-function electrode composed of Co ₃ Mo particles interfaced with CoMoO ₃ sheets, showing it can outperform conventional Pt/C and RuO ₂ catalysts in alkaline full-cell electrolysis at high current relate its architecture to electrocatalytic behavior? |
| How does the paper that investigates how strong electronic interactions at the junction between Co ₃ Mo nanoparticles and a porous CoMoO ₃ matrix promote efficient hydrogen evolution by enhancing water splitting kinetics explain its findings? |
| How does the paper that constructs a vertically aligned CoMoS ₄ nanosheet layer over a sulfide-rich Ni ₃ S ₂ underlayer and demonstrates their cooperative effect on boosting oxygen evolution in alkaline solution explain its findings? |
| What evidence does the paper that explores a hybrid catalytic platform where Ni ₃ S ₂ improves charge transport to CoMoS ₄ nanosheets, enabling low-voltage water electrolysis in both HER and OER regimes present? |
| How does the paper that fabricates partially phosphidized cobalt nanowires with internal pores and examines how their 3D morphology influences catalytic behavior in acidic and basic water splitting explain its findings? |
| How does the paper that fine-tunes the crystallinity and surface defects of NiCo ₂ O ₄ nanorods through sulfur treatment, and evaluates their bifunctional catalytic response in water splitting explain its findings? |
| How does the paper that links the presence of abundant grain boundaries and sulfur doping in spinel nanorods to improvements in charge transfer efficiency during electrolysis explain its findings? |
| How does the paper that embeds graphene-based quantum structures into nickel–cobalt phosphide nanosheets to manipulate charge flow pathways and achieve high-rate hydrogen production explain its findings? |
| What evidence does the paper that examines the synergy between graphene quantum dots and phosphide nanosheets in enabling efficient overall water electrolysis compared to oxide or wire-type analogs present? |
| How does the paper that shows how brief ultrasonic treatment alters the structure of NiFe LDH nanosheets, introducing defects and spacing that reduce onset potential for oxygen evolution explain its findings? |
| How does the paper that associates sonochemically induced lattice distortions in NiFe hydroxides with improved kinetics and a favorable change in the rate-limiting step for OER explain its findings? |
| How does the paper that identifies low-temperature-derived Co ₃ O ₄ microspheres with fine nanostructure as superior OER catalysts due to their abundant surface cobalt sites explain its findings? |
| How does the paper that reveals how Co ₃ O ₄ nanoparticles prepared under mild heat retain small crystal sizes, which contribute to higher OER efficiency without requiring composite strategies explain its findings? |
| How does the paper that combines layered NiFe hydroxides with a hybrid support of graphdiyne and graphene, showing that this interface engineering significantly boosts alkaline OER performance explain its findings? |
| How does the paper that contrasts the catalytic behavior of NiFe-LDH on various carbon supports and finds that coupling to graphdiyne–graphene hybrids enables both fast kinetics and long-term stability explain its findings? |
| How does the paper that builds nanoneedle-like CoMoO ₄ assemblies and links their porous internal architecture to enhanced OER and supercapacitor behavior through rapid electron-ion transport explain its findings? |
| How does the paper that compares hierarchical CoMoO ₄ with other oxide catalysts and attributes its superior OER activity to the nanosheet-based needle structure and high surface exposure explain its findings? |
| How does the paper that links the bifunctional water-splitting ability of Ni–Mo nitride heterostructures to charge redistribution at the metal/nitride interfaces together with fast electron transport provided by nitrogen-doped carbon nanotube scaffolds on carbon cloth explain its findings? |
| Which synergistic effects are detailed in the paper that describes a self-supporting electrode where encapsulated Ni/MoN clusters and a three-dimensional CNT network jointly enable the same substrate to drive both hydrogen and oxygen evolution under alkaline conditions? |
| How does the paper that attributes superior oxygen evolution kinetics of cobalt oxide on N-CNTs to ammonia-driven nitrogen incorporation plus partial lattice reduction, which together improve conductivity and promote in-situ transformation into active oxyhydroxide layers explain its findings? |
| How does the paper that contrasts NH ₃ -treated and H ₂ -treated CoOx/NCNT catalysts, showing that surface nitrogen enhances hydrophilicity and long-term stability even though cobalt appears in a lower |

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| formal oxidation state after the ammonia step explain its findings? |
| How does the paper that designs seaweed-like $\text{Ni}_3\text{S}_2@\text{MoS}_2@\text{Ni}_3\text{Si}_2$ hybrids whose intertwined sulfide interfaces cooperate with a conductive silicide backbone to minimise charge-transfer resistance while providing abundant edge sites for both half-reactions explain its findings? |
| How does the paper that achieves simultaneous hydrogen and oxygen catalysis by in-situ growing hierarchical sulfide–silicide structures on nickel foam, thereby combining mechanical adhesion with accelerated gas release pathways explain its findings? |
| How does the paper that fabricates defect-rich Co carbonate hydroxide cores enveloped by CoSe nanosheets, and explains how their heterointerface together with a nickel-foam current collector boosts electron migration during overall water splitting explain its findings? |
| How does the paper that employs a two-step hydrothermal route to engineer oxygen-vacancy-containing $\text{CoCO}_3 \cdot 0.5\text{H}_2\text{O}@\text{CoSe}$ nanowires whose synergistic lattice strain and conductive support underpin robust bifunctional performance explain its findings? |
| How does the paper that reports an unusual trend in $\text{Co}_2\text{Fe-LDH}/\text{N-graphene}$ hybrids where increasing hydroxide loading simultaneously raises catalytic activity and charge-transfer resistance, an effect traced to hydrophilic LDH layers preventing graphene restacking explain its findings? |
| How does the paper that confirms by rotating-ring–disk studies that the most active LDH/graphene composite follows a four-electron oxygen pathway despite exhibiting higher interfacial impedance than leaner formulations explain its findings? |
| How does the paper that introduces a chemically robust bimetallic squarate MOF whose one-dimensional Ni–Fe hydroxide strips offer open channels for electrolyte diffusion while simultaneously acting as built-in catalytic sites explain its findings? |
| How does the paper that shows tuning the Ni:Fe ratio in a squarate framework optimises both structural stability and electron transport, enabling a porous MOF to rival layered double hydroxides in oxygen evolution explain its findings? |
| How does the paper that demonstrates trivalent iridium dopants donate more electron density to neighbouring oxygen in NiFe-LDH than tetravalent iridium, thus accelerating alkaline water dissociation and hydrogen desorption explain its findings? |
| How does the paper that generalises the above valence-state effect to ruthenium and platinum dopants, concluding that oxidation state selection is a critical design lever for layered hydroxide electrocatalysts explain its findings? |
| How does the paper that upcycles yeast biomass into multi-heteroatom-doped carbon hosting both ruthenium single atoms and nanoparticles, enabling sustained solar-driven water splitting through coupled $\text{Fe}^{2+}/\text{Fe}^{4+}$ redox chemistry at the anode explain its findings? |
| How does the paper that attributes the low interfacial resistance of an $\text{Fe}_3\text{O}_4@\text{carbon}$ anode to synergistic interactions with a doped-carbon matrix, resulting in stable outdoor operation without noble-metal oxides explain its findings? |
| How does the paper that constructs sub-microwires comprising a metallic MoO_2 core clad with MoS_2 nanosheets and Ni_2P nanoparticles, so that nested electron pathways and multi-interface coupling deliver bifunctional catalysis explain its findings? |
| How does the paper that explains how temperature-programmed sulfuration followed by phosphidation transforms nickel molybdate into a tri-component hybrid whose individual phases collectively address conductivity, active-site density and reaction kinetics explain its findings? |
| How does the paper that investigates how Fe incorporation into NiS_2 affects the metallic nature and suppresses thick passivation layer formation during OER cycles explain its findings? |
| What evidence does the paper that examines the role of Fe–S bond shortening in improving the structural resilience of NiS_2 -based electrocatalysts under alkaline OER conditions present? |
| How does the paper that utilizes molten KSCN salt and surface corrosion to fabricate amorphous-crystalline hybrid NiFe sulfide catalysts for high current density OER explain its findings? |
| What evidence does the paper that explores the synergistic interplay between nanoglass-structured FeNi_2S_4 and amorphous NiFe–LDH in sustaining industrial-grade OER at elevated temperature and electrolyte strength present? |
| How does the paper that uses carbon derived from acid-treated sucrose to enhance Co_3O_4 composite performance for the oxygen evolution reaction explain its findings? |
| How does the paper that designs ternary $\text{CoP}_{2x}\text{Se}_2(1-x)$ nanowires through dual doping to improve water splitting performance in a single alkaline cell explain its findings? |
| How does the paper that reports how fine-tuned P-to-Se substitution in cobalt-based ternary nanowires affects HER and OER activities symmetrically in dual-electrode configurations explain its findings? |
| How does the paper that employs etching followed by phosphorus doping to produce Fe-modified |

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| CoP nanowires optimized for dual HER and OER performance explain its findings? |
| How does the paper that correlates the optimal Fe doping ratio in Co-based phosphide nanowires with minimized overpotential in both cathodic and anodic reactions explain its findings? |
| How does the paper that demonstrates the stabilization of hollow CoP/MnO nanofibers through controlled phosphidation of MnCo ₂ O ₄ intermediates for OER durability explain its findings? |
| How does the paper that attributes enhanced OER activity to the internal structure of CoP/MnO nanofibers designed for extended cycling stability explain its findings? |
| How does the paper that introduces fluorine as a dopant to generate oxygen vacancies and modify the band structure of cobalt molybdate nanosheets for OER catalysis explain its findings? |
| How does the paper that shows how F-induced vacancy engineering and Mo 4d orbital tuning synergistically boost OER kinetics in CoMoO ₄ explain its findings? |
| How does the paper that constructs a 3D Ni ₂ P–MoS ₂ heterostructure on carbon cloth using a two-step conversion process to optimize bifunctional catalytic activity explain its findings? |
| How does the paper that attributes exceptional HER and OER performance to interface effects in vertically grown Ni ₂ P–MoS ₂ nanosheet arrays explain its findings? |
| How does the paper that designs okra-shaped Cu-doped CoP/Co ₃ O ₄ hollow nanotube arrays and evaluates their full-cell water splitting efficiency explain its findings? |
| What evidence does the paper that explores the dual role of vanadium in simultaneously reducing Pt clusters and enhancing charge transfer in NiFe LDH for water splitting present? |
| Which factors does the paper that analyzes how vanadium shifts Ni's d-band center to balance adsorption–desorption energetics during OER and HER in a bifunctional electrocatalyst identify? |
| What mechanistic explanation does the paper that discusses how nickel incorporation transforms FeS ₂ into a semimetal with improved water affinity for oxygen evolution catalysis provide? |
| How does the paper that evaluates a yolk-shell Fe-based electrocatalyst undergoing structural reformation into NiFeOOH during alkaline oxygen evolution explain its findings? |
| How does the paper that investigates the impact of gold nanoparticles on promoting NiFe layered hydroxide arrays for high-current OER in alkaline base explain its findings? |
| How does the paper that links the enhanced oxygen evolution activity of a NiFe LDH electrode to the formation of Ni ³⁺ species induced by gold decoration explain its findings? |
| How does the paper that correlates superexchange interactions in Ni–Fe hydroxides with their boosted oxygen evolution efficiency in alkaline solution explain its findings? |
| How does the paper that explains the superior electrocatalytic performance of a NiFe layered hydroxide with 1.5 Ni/Fe ratio via magnetic and DEMS analysis explain its findings? |
| How does the paper that attributes enhanced oxygen evolution kinetics to a 3D-printed stainless-steel cone array coated with NiCo ₂ S ₄ nanoneedles explain its findings? |
| How does the paper that demonstrates how structural design of metal support enables 21-fold improvement in electroactive area for water splitting explain its findings? |
| Which factors does the paper that analyzes how high-valent cobalt doping in Fe–Ni hydroxides alters the electronic structure and enhances OER kinetics identify? |
| How does the paper that evaluates a nanoneedle-based Fe–Ni–Co hydroxide electrode integrated with FeSe ₂ /C for supercapacitor and oxygen evolution explain its findings? |
| How does the paper that develops hierarchical NiFeV hydroxide nanotubes with V-induced charge redistribution for improved oxygen evolution performance relate its architecture to electrocatalytic behavior? |
| How does the paper that converts NiFeV hydroxide into phosphide while preserving its nanotube morphology for enhanced alkaline OER explain its findings? |
| How does the paper that reports a ternary aerogel electrode where charge separation is facilitated by codoped graphene, enabling both HER and OER under basic conditions explain its findings? |
| How does the paper that details an in situ hybrid of WSe ₂ and NiFe-LDH assembled on N,S-rGO framework using a hydrothermal method for bifunctional energy devices explain its findings? |
| What mechanistic explanation does the paper that discusses HER and UOR activity enhancement through tailoring Co/Mo ratios in vertically grown sulfide nanosheets provide? |
| What evidence does the paper that explores how Mo incorporation into CoS ₂ reshapes surface morphology and boosts alkaline electrocatalysis present? |
| How does the paper that investigates OER performance improvement through direct integration of a trimetallic hydroxide cluster onto Ti ₃ C ₂ MXene explain its findings? |
| How does the paper that attributes enhanced oxygen evolution activity to increased electron density near the Fermi level via metal–MXene interaction explain its findings? |
| How does the paper that shows SAC performance maximization by tuning Ni/Fe mass ratio below a critical threshold during carbon-supported catalyst formation explain its findings? |

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| How does the paper that presents carbon-supported NiFe single-atom catalysts fabricated via one-step pyrolysis and optimized for low-resistance OER explain its findings? |
| How does the paper that leverages composition-gradient NiFe hydroxides to engineer continuous electron pathways and boost OER activity explain its findings? |
| Which synergistic effects are detailed in the paper that describes a hydrothermal synthesis where trisodium citrate promotes gradient nanosheet formation on Ni foam for electrocatalysis? |
| How does the paper that introduces a one-pot embedding of Pt nanoparticles into Ni-Fe Prussian blue analog nanocubes for bifunctional water splitting explain its findings? |
| How does the paper that reports a porous nanocube electrocatalyst where acid etching enhances surface area for both HER and OER explain its findings? |
| How does the paper that develops a self-supported bifunctional electrode via phosphidation of oxidized cobalt foil for water splitting relate its architecture to electrocatalytic behavior? |
| How does the paper that identifies P-top sites in Co ₂ P as active centers for HER using both experimental and DFT analyses explain its findings? |
| How does the paper that fabricates TiO ₂ -based electrocatalysts where surface Zn dissolution triggers a self-optimizing structure for chlorate production explain its findings? |
| How does the paper that enhances CER selectivity via co-deposition and post-treatment of Zn-Ru-Ti alloys leading to a rough, porous TiO ₂ matrix explain its findings? |
| How does the paper that constructs ~50 nm hollow nanospheres of nickel oxysulfide through solvothermal growth for bifunctional electrocatalysis explain its findings? |
| How does the paper that assesses HER/OER activity of fullerene-mimetic Ni-based nanospheres supported on nickel foam explain its findings? |
| How does the paper that fabricates FCC-Ni/NiS heterostructures within N,S-doped rGO via stepwise annealing of coordination polymer/GO hybrids explain its findings? |
| How does the paper that attributes enhanced OER activity to multiphase interfaces and nanoscale layering in a hybrid Ni-based composite explain its findings? |
| How does the paper that demonstrates how incorporating a fourth transition metal improves the reaction rate at high current densities in a FeCoNi-based alloy explain its findings? |
| How does the paper that achieves phosphide formation without using hazardous phosphorus donors by transforming LDH nanosheets in hydrogen atmosphere explain its findings? |
| How does the paper that relates electrocatalytic activity to spin configuration and electron redistribution at Ni-based active centers explain its findings? |
| How does the paper that shows OER efficiency peaks at specific d-band values when doping Ni-MOFs with various 3d metals explain its findings? |
| How does the paper that constructs hollow tri-metal selenide nanostructures by leveraging template-directed carbon frameworks explain its findings? |
| How does the paper that achieves dual electrocatalysis by integrating Cu, Ni, and Co into selenide nanosheets supported on nitrogen-rich scaffolds explain its findings? |
| How does the paper that identifies 200 °C as the optimal condition for achieving low overpotential in Mo-doped Ni ₃ S ₂ grown on conductive substrates explain its findings? |
| How does the paper that attributes OER activity enhancement to thermally induced oxygen vacancy formation in nanobelt catalysts explain its findings? |
| How does the paper that tunes oxygen vacancy levels in spinel-type nanobelts through inert atmosphere annealing at different temperatures explain its findings? |
| How does the paper that explains OER enhancement through synergistic interplay in a nickel oxide-phosphide core-shell nanosheet architecture explain its findings? |
| How does the paper that synthesizes hollow Co-Fe phosphide microtubes through multistep conversion from metal-organic precursors explain its findings? |
| How does the paper that applies a urea-based method to produce conductive hafnium nitride nanoparticles for oxygen electrocatalysis explain its findings? |
| How does the paper that emphasizes long-term catalyst durability in alkaline OER using a metal nitride not previously tested explain its findings? |
| How does the paper that constructs high-performing anodes by directly converting Ni foam with iron and vanadium ions without using deposition techniques explain its findings? |
| How does the paper that investigates seawater electrolysis using a hierarchical IrO ₂ @MnO ₂ structure supported by reduced graphene oxide explain its findings? |
| How does the paper that evaluates FeNi ₃ @Ni nanoparticles for durability in AMF-enhanced electrolysis via ILTEM and in situ XRD explain its findings? |
| What evidence does the paper that explores the long-term crystallographic transformations of FeNi ₃ @Ni under reductive and oxidative conditions up to 600°C present? |

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| How does the paper that attributes enhanced OER activity to a synergistic interface between FeOOH and hollow NiCoP/C nanocages explain its findings? |
| How does the paper that demonstrates electron redistribution at a coupling interface between FeOOH and NiCoP/C improves OER intermediate adsorption explain its findings? |
| How does the paper that achieves dual HER and OER activity using porous nitrogen-doped carbon nanofibers embedded with cobalt nanoparticles explain its findings? |
| How does the paper that uses an electrospinning method followed by acid etching to create porous Co-PNCNFs with high OER current density explain its findings? |
| How does the paper that develops amorphous iron oxide nanosheet arrays via electrochemical desulfurization for self-supported OER electrodes relate its architecture to electrocatalytic behavior? |
| How does the paper that reports enhanced OER activity after long-term operation of FeOx nanosheets grown on carbon cloth explain its findings? |
| How does the paper that enhances Ni(OH) ₂ OER performance by pillaring it with zero-dimensional polyoxovanadate clusters explain its findings? |
| How does the paper that forms a 2D/0D nanohybrid of Ni(OH) ₂ and polyoxovanadates via chemical solution growth in decarbonated water explain its findings? |
| How does the paper that synthesizes Fe ₂ Co ₈ HCF nanospheres with a core-shell structure showing bifunctional water splitting activity at 1.63 V explain its findings? |
| How does the paper that attributes high OER and HER performance to interfacial strain and electronic redistribution in Fe ₂ Co ₈ HCF core-shell catalysts explain its findings? |
| How does the paper that investigates how increasing Co ₂ Fe LDH loading on N-doped graphene paradoxically raises charge transfer resistance while enhancing OER activity explain its findings? |
| How does the paper that attributes improved OER performance of Co ₂ Fe LDH–N-graphene hybrids to inhibition of graphene stacking and uniform LDH dispersion explain its findings? |
| What evidence does the paper that fabricates flower-like cobalt sulfide nanostructures, couples them with acid-functionalized multi-walled carbon nanotubes through ultrasonic dispersion, and ascribes the improved oxygen evolution to enhanced interfacial electronic coupling present? |
| How does the article that engineers defect-rich NiO sheaths around NiMoO ₄ nanorods, enabling a three-stage Fe capture process (adsorption, migration, and impregnation) that reconstructs the surface into active oxyhydroxide layers explain its findings? |
| How does the study that varies the Fe/Ni ratio in a NiMoO ₄ @NiO heterostructure and correlates operando X-ray absorption evidence of electronic tuning with accelerated lattice-oxygen-mediated catalysis in alkaline media explain its findings? |
| What evidence does the study that reports an ultrathin anthraquinone polymer film draped over Ni ₃ S ₂ nanosheets forming a “3D-stretched” architecture whose long-term alkaline durability is linked to interfacial π–d conjugation present? |
| How does the study that discusses how the π–d conjugation in polymer-metal sulfide interactions revealed by operando Raman and DFT analysis contributes to its electrocatalytic performance explain its findings? |

Supplementary Table 3. Descriptive questions for OER qualitative evaluation with RAGAS (n=202). All questions are formulated to assess scientific knowledge through free-form responses.