An Explainable Conversational AI Framework for the Discovery of Cobalt Electrocatalysts in Industrial Water Electrolysis

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1. Introduction

Sustainable hydrogen generation relies on proton exchange membrane (PEM) electrolyzers, but their widespread commercialization is hindered by scarce, costly noble-metal catalysts like RuO_2 and IrO_2 [1]. Consequently, earth-abundant cobalt spinel oxides (Co_3O_4) have garnered attention for their economic viability and adjustable electronic characteristics [1,2]. Although recent multi-elemental doping efforts boost catalytic efficacy and lifespan, enhancements fall short of industrial requirements. Furthermore, traditional trial-and-error methods focus on narrow compositional subsets, failing to systematically understand stability-activity trade-offs across vast chemical domains.

To overcome this, we propose an explainable conversational artificial intelligence (AI) framework to navigate the expansive multi-metallic spinel space. Leveraging curated experimental data, this AI agent accurately forecasts catalytic durability and activity, bridging the gap between dopant combinations and structural or electronic shifts. Moving beyond black-box prediction [3], our intuitive system yields quantitative, cost-constrained design guidelines to logically navigate intricate material libraries. Guided by this model, we synthesized an optimal high-entropy Co_3O_4 (HE-Co_3O_4) that vastly outperforms conventional oxides in activity and durability, proving its capability for sustained, noble-metal-free operation in practical PEM devices. This outlines a generalized strategy for identifying high-performing materials in massive compositional spaces.

2. Results and Discussion

2.1 ML-guided discovery and combinatorial screening

We established an empirical dataset of 30 distinct cobalt spinels, sampled from over 4,368 potential multi-elemental combinations for broad chemical space coverage (**Fig. 1a**). We synthesized and evaluated these candidates' structural signatures via X-ray diffraction (XRD) and X-ray photoelectron spectroscopy (XPS), while quantifying electrochemical performance through oxygen evolution reaction (OER) overpotential and chronopotentiometric durability testing. This foundational data trained our machine learning architecture to extrapolate stability and activity across the combinatorial space (**Fig. 1b**). Within this mapping, the explainable AI organized candidates into interpretable clusters, quantitatively linking dopant shifts to structural/electronic transformations and establishing cost-aware design rules. Guided by these insights, we identified and experimentally verified a multi-metallic spinel explicitly optimized for maximum OER activity and operational lifespan.

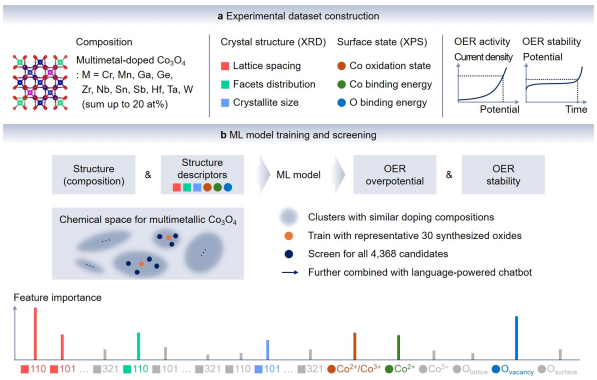

Fig. 1: ML-guided workflow. a, Experimental dataset construction. b, Model training and screening.

2.2 Explainable conversational interface for material optimization

Following computational screening, the data matrices were ingested into a customized conversational interface, allowing researchers to query the database using natural language. Engineered using the GPT-4.1 architecture with a FAISS-based vector retrieval system and a temperature setting of 0.25, this agent guarantees deterministic, scientifically precise outputs for high-dimensional materials data. Upon requesting the ideal formulation for maximizing performance, the agent instantly retrieved the optimal high-entropy spinel configuration (**Fig. 2**). Crucially, the system demonstrates explainabil-

ity by elucidating the underlying structural descriptors driving predictions, pointing out how variations in lattice dimensions, surface oxidation states, and oxygen vacancies dictate catalyst behavior. The AI also delineates element-specific influences, explaining mechanisms by which individual dopants alter binding affinities and defect formations to enhance durability. Incorporating real-time commodity pricing enables budget-restricted searches; for example, the agent proposed an alternative formulation slashing raw material expenses by over one-third while marginally sacrificing stability.

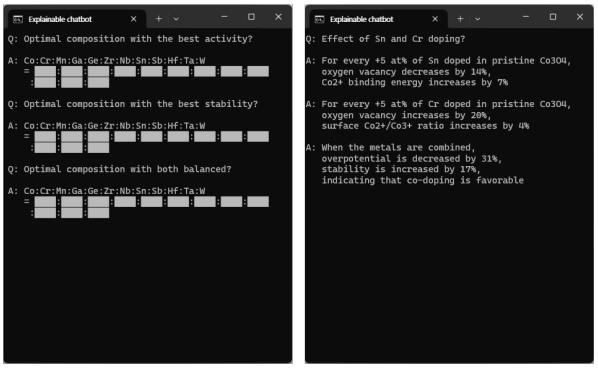

Fig. 2: Explainable AI-guided material design. Interactive queries and design rules generated by the GPT-4.1-powered conversational agent.

2.3 Experimental validation toward industrial application

To substantiate AI-generated predictions, HE-Co_3O_4 underwent experimental validation. Initial sol-gel synthesized half-cell tests in 0.5 M H_2SO_4 confirmed HE-Co_3O_4 delivered exceptional OER performance, achieving an impressively low overpotential and extended durability compared against screened candidate oxides (**Fig. 3a**). Structural characterization confirmed multi-metallic doping modulated critical surface properties while preserving the core spinel lattice. To evaluate commercial viability, HE-Co_3O_4 was fabricated using a zeolitic imidazolate framework (ZIF) templating method, yielding a robust microscopic architecture. This optimized catalyst demonstrated exceptional long-term endurance, sustaining 500 mA cm^{-2}_{disk} for over 250 hours within a PEM electrolyzer setup (**Fig. 3b**). Integrating this explainable AI interface with macroscopic industrial application bridges half-cell screening and industrial-level validation, overcoming traditional longevity barriers of platinum-group-metal-free electrodes in scalable applications [1,2].

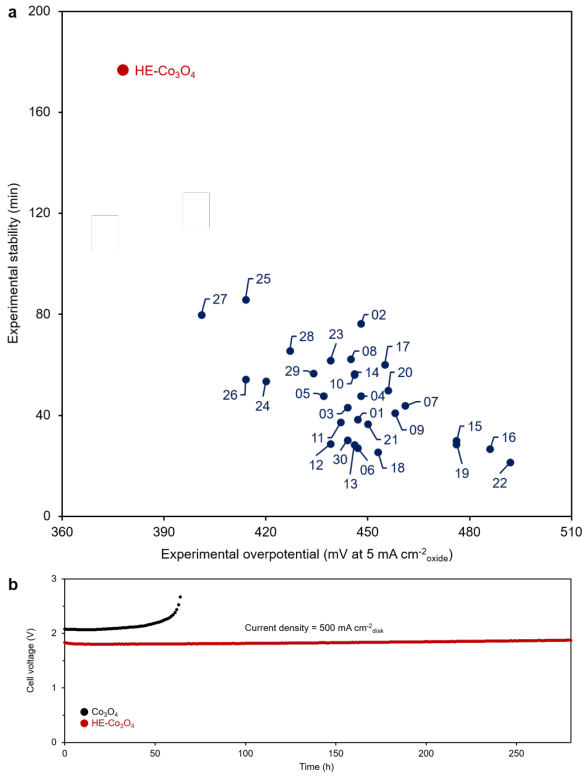

Fig. 3: Experimental validation. a, OER performance of HE-Co_3O_4 vs. screened oxides in 0.5 M H_2SO_4. b, PEM water electrolyzer stability of HE-Co_3O_4.

3. Conclusion

This research merges machine learning with an explainable conversational AI agent to explore immense compositional spaces. By translating complex structure-property relationships into quantitative design parameters, the framework empowers researchers to rapidly identify efficient, cost-effective materials. This system harmonizes deep predictive capabilities with human-readable interpretability, accelerating the discovery of advanced materials.

Acknowledgments

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