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Application of Diatomic Electrocatalysts in Oxygen Reduction

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Abstract. These days, the world really needs sustainable energy storage solutions to deal with energy shortages and environmental problems. Against that background, zinc-air batteries (ZABs) have become a pretty promising technology, mainly because they offer a high theoretical energy density and zinc is abundant. But there's a catch—their performance gets held back by the slow kinetics of the oxygen reduction reaction (ORR) at the cathode, plus the Pt-based catalysts people often use are quite expensive. So, in this study, we looked at how well a diatomic FeCo-NC electrocatalyst works for the ORR in ZABs. We made this catalyst using a bimetallic zeolitic imidazolate framework (ZIF-8/ZIF-67) as a precursor and then did a thermal pyrolysis method. When we tested it electrochemically, the FeCo-NC catalyst showed really good ORR activity in alkaline media—it gave a half-wave potential of 0.875 V and a limiting current density of 5.430 mA cm^{-2}, numbers that are quite close to what commercial Pt/C gives. Our mechanistic studies also confirmed that the reaction mainly follows a four-electron transfer pathway, and the reaction kinetics look favorable too. So, this work shows that atomically dispersed bimetallic catalysts could be an efficient and cost-effective alternative to noble-metal catalysts for advanced energy conversion devices like zinc-air batteries. It also offers some ideas for where future research could go, especially on precise synthesis and getting a better handle on the mechanisms.

Keywords: Oxygen reduction reaction, Catalyst, Reaction Kinetics

1. Introduction

Ever since the 21st century started, society has been developing fast, and that's made global energy shortages and environmental pollution worse and worse. Our heavy dependence on fossil fuels hasn't just deepened the energy crisis; it has also pushed up greenhouse gas emissions, which further harms the environment [1-4]. Plus, with China now having its "carbon peak and carbon neutrality" strategic goals, switching from traditional fossil fuels to clean energy has become an urgent task. But renewable energy sources come and go—they're intermittent and fluctuate—so we have to come up with efficient energy storage technologies [5-8]. The lithium-ion batteries we use today have their own issues: resources are scarce and there are safety concerns, so they're not really suitable for grid-scale storage. That's why developing an electrochemical energy storage system that gives both high energy density and low cost has turned into a key research goal.

Among all the energy storage technologies out there, zinc-air batteries have drawn a lot of attention because they bring some unique advantages to the table. Their theoretical energy density

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can go up to 1,353 Wh/kg, which is about five times that of lithium-ion batteries. Zinc resources are plentiful too—China's zinc ore reserves alone make up about 20 % of the world's total, and that share has been growing each year; in fact, zinc reserves are more than fifty times larger than lithium reserves. Cost-wise, zinc is pretty economical: the material cost for zinc batteries is roughly one-third of what lithium batteries cost. And the byproduct, zinc oxide, isn't toxic, so it's environmentally friendly [9]. Zinc batteries also don't have thermal runaway risks, and their electrolyte is a neutral water solution that can be recycled at over 95 %. However, the slow kinetics of the cathodic oxygen reduction reaction end up hurting the battery's electrochemical performance quite a bit [10]. To make matters worse, the Pt/C catalyst that's widely used is both scarce and expensive, which really limits how far it can be commercialized. That's why a lot of researchers are now looking at transition metals as possible alternatives to those precious metal catalysts..

If you can disperse metal atoms at the atomic level on a carrier surface, you can achieve high activity and stability. Single-atom catalysts do this by anchoring metal atoms onto the carrier surface[11-13], which gives 100 % atom utilization. But they only have single active sites, and because their surface energy is high, those atoms tend to clump together. Their electronic structure is also pretty symmetric, which ends up suppressing the adsorption and activation of oxygen intermediates. Compared to single-atom catalysts, dual-atom catalysts consist of two adjacent metal atoms. The metal atoms in these catalysts are highly dispersed, so you avoid the nanoparticle agglomeration problem, and you maximize the use of active sites. There's also electron transfer happening between the dual-atom sites, and that electron transfer helps optimize the adsorption of reactants and the formation of intermediates, stabilizing them and lowering the reaction energy barrier [14-17]. So, we decided to take advantage of the synergistic effects that bimetallic catalysts can offer, so we could optimize the reaction pathway. In this work, we used a zeolitic imidazolate framework (ZIF) with high porosity as a precursor, and then through high-temperature pyrolysis we prepared a catalyst with atomically dispersed metal sites[18-24]. Our aim was to get past the kinetic bottleneck that the cathode reaction faces in zinc-air batteries, and at the same time, offer some new directions for designing cathode materials for zinc-air batteries. This research hopefully gives a fresh technical route for clean energy storage.

2. Material preparation

2.1. Preparation of ZIF-67

We first weighed out a certain amount of $Co(NO_3)_2 \cdot 6H_2O$ and dissolved it in 250 mL of methanol. After sonicating it for 1 minute, we got a clear pink solution with a concentration of 0.04 M. Then we weighed out a certain amount of 2-methylimidazole and dissolved that in 250 mL of methanol too. Next, we poured the cobalt nitrate solution into the 2-methylimidazole solution, put the mix on a magnetic stirrer, and let it stir for 4 hours. When the reaction was done, the solution had become a deep purple suspension. We then centrifuged it at 8000 rpm for 5 minutes to collect the precipitate. That precipitate got washed three times with methanol, and each time we centrifuged it again to remove any unreacted raw materials and solvents. Finally, we put the purple precipitate into a vacuum drying oven and dried it at 60 °C for 12 hours, and that's how we got the ZIF-67 powder.

2.2. Preparation of ZIF-8

We weighed out a certain amount of $Zn(NO_3)_2 \cdot 6H_2O$ and dissolved it in 250 mL of methanol. After sonicating for 1 minute, we got a clear pink solution at 0.04 M. Then we weighed out a certain

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amount of 2-methylimidazole and dissolved it in 250 mL of methanol. We poured the zinc nitrate solution into the 2-methylimidazole solution and stirred it on a magnetic stirrer for 4 hours. Once the reaction finished, the solution also turned into a deep purple suspension. We centrifuged it at 8000 rpm for 5 minutes to collect the precipitate, washed it three times with methanol, and centrifuged again to get rid of any unreacted materials and solvents. Then we put the purple precipitate into a vacuum drying oven and dried it at 60 °C for 12 hours, which gave us the ZIF-8 powder.

2.3. Preparation of the bimetallic catalyst FeCo-NC

We took 0.2 g, 0.4 g, and 0.6 g of the ZIF-8 powder respectively and added each to the precursor solution that we normally use for preparing ZIF-67 (that solution is a mixture of cobalt nitrate and 2-methylimidazole). Then we stirred the mixture for 4 hours. After the reaction was done, we got a purple suspension. That suspension was centrifuged at 8000 rpm for 5 minutes so we could collect the precipitate. We washed the precipitate three times with methanol and once with ethanol, and then we put the purple precipitate into a vacuum drying oven to dry at 60 °C for 12 hours. That gave us the ZIF-8/ZIF-67 composite material. Next, we placed that composite material into a tube furnace and carbonized it at 900 °C. After the first carbonization, we added a small amount of $Fe(NO_3)_2 \cdot 6H_2O$ to the material and put it back into the tube furnace for a second carbonization. That finally gave us what we wanted—the bimetallic FeCo-NC catalyst.

3. Results and discussion

We systematically evaluated the ORR catalytic performance of the bimetallic FeCo-NC catalyst in an alkaline medium using a rotating disk electrode (RDE) setup. As is evident from the cyclic voltammetry (CV) profiles presented in Figure 1, under an N-saturated atmosphere, no discernible ORR reduction peak was observed. From this, the inference follows that non-faradaic processes or side reactions capable of being misread as ORR activity were absent. Under an O-saturated environment, by contrast, a pronounced and well-defined cathodic peak emerged, indicating that oxygen reduction was indeed taking place. For FeCo-NC, the peak potential reached 0.852 V versus RHE, a value higher than the 0.837 V reported for commercial 20% Pt/C catalysts under comparable test conditions [25]. That positive displacement of the reduction potential points to a lower overpotential and more favorable ORR kinetics for FeCo-NC. Taken together, these observations indicate that FeCo-NC not only promotes the oxygen reduction reaction in alkaline media, but also exhibits exceptional electrocatalytic activity, thereby underscoring its promise as an efficient and cost-effective substitute for platinum-based catalysts in advanced energy-conversion systems.

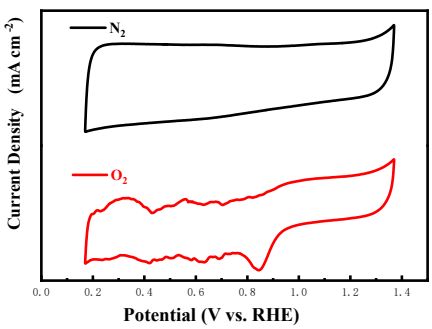


Figure 1. Cyclic voltammetry curve of the diatomic catalyst FeCo-NC

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To secure a broader comparison of ORR electrocatalytic behavior, linear sweep voltammetry (LSV) measurements were subsequently conducted for different catalysts at a rotation speed of 1600 rpm with a rotating disk electrode. The corresponding results appear in Figure 2. Across the LSV curves, marked differences were observed in both the limiting diffusion current density (J_L) and the half-wave potential (E/), parameters that bear directly on catalytic activity and efficiency. Specifically, the J_L values obtained for Co-NC-9, Co-NC-18, Co-NC-36, and FeCo-NC were 4.725 mA cm, 5.465 mA cm, 5.355 mA cm, and 5.430 mA cm, respectively. Their associated half-wave potentials were 0.838 V, 0.845 V, 0.848 V, and 0.875 V.

Among the tested samples, the bimetallic FeCo-NC catalyst delivered the strongest overall performance. Most positive was its half-wave potential, 0.875 V, and its limiting current density remained high at 5.430 mA cm; taken together, these values approach those typically observed for benchmark commercial Pt/C catalysts. The data therefore indicate that the ORR electrocatalytic performance of FeCo-NC has essentially reached the Pt/C level and, when onset and half-wave potentials are considered, may even be marginally superior. A reasonable basis for this enhanced activity lies in the deliberate incorporation of iron, which facilitates the formation of synergistic bimetallic Fe-Co sites within the nitrogen-doped carbon matrix. Through that bimetallic interaction, the density and accessibility of active sites are increased, while the local electronic structure is simultaneously optimized; accelerated charge-transfer kinetics and improved oxygen adsorption and activation follow.

By comparison, the monometallic cobalt-based catalysts in the Co-NC series possess a more uniform, more symmetric electronic environment, and such an environment appears less favorable for effective oxygen binding and the subsequent reduction steps. Their ORR performance is therefore comparatively weaker. Within the Co-NC framework, iron incorporation effectively tunes the catalytic interface, yielding improved overall reactivity and durability. In that respect, the present results bring the role of bimetallic synergy into sharp focus for the rational design of high-performance non-precious metal catalysts intended for alkaline fuel cells and related energy technologies.

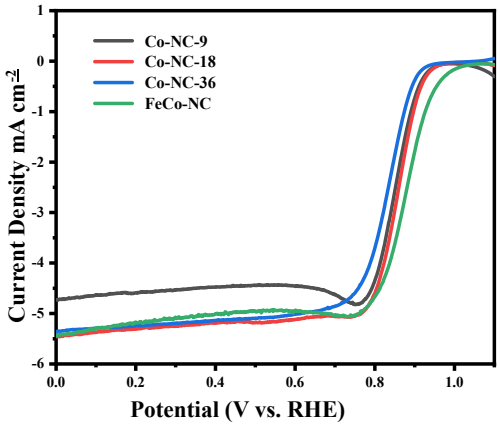


Figure 2. Linear sweep voltammetry curves of ORR for different catalysts

To dig deeper into the ORR kinetics and the electron transfer mechanism for the FeCo-NC catalyst, we systematically ran LSV tests over a range of rotation speeds from 900 to 2500 rpm. It's pretty well known that turning up the rotation rate makes dissolved O_2 diffuse faster toward the electrode surface, which enhances mass transport and helps supply the reactant more efficiently. As

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Figure 3a clearly shows, the LSV curves we got depend strongly on rotation speed: the limiting diffusion current density goes up noticeably as we increase the rotation speed, which matches the idea that higher hydrodynamic conditions improve convective mass transfer. To quantitatively evaluate the electron transfer mechanism that governs the ORR process, we did Koutecky-Levich (K-L) analysis based on the LSV data collected at different rotation rates. The K-L plots we built at various electrode potentials showed excellent linearity and parallelism, which indicates that the reaction follows first-order kinetics with respect to dissolved oxygen concentration. As presented in Figure 3b, the calculated electron transfer number (n) came out to be about 4.0 per oxygen molecule. That gives us solid proof that the ORR on FeCo-NC mainly goes through a highly efficient four-electron transfer pathway. This pathway reduces oxygen directly to water, unlike the two-electron route that makes intermediate hydrogen peroxide (H_2O_2). Having the four-electron mechanism dominate not only improves the overall catalytic efficiency but also cuts down a lot on the formation of corrosive peroxide species, which lowers the risk of electrode degradation and catalyst instability. So, the FeCo-NC catalyst ends up showing better durability and operational stability, making it a promising candidate for alkaline energy conversion devices like fuel cells and metal-air batteries [26, 27].

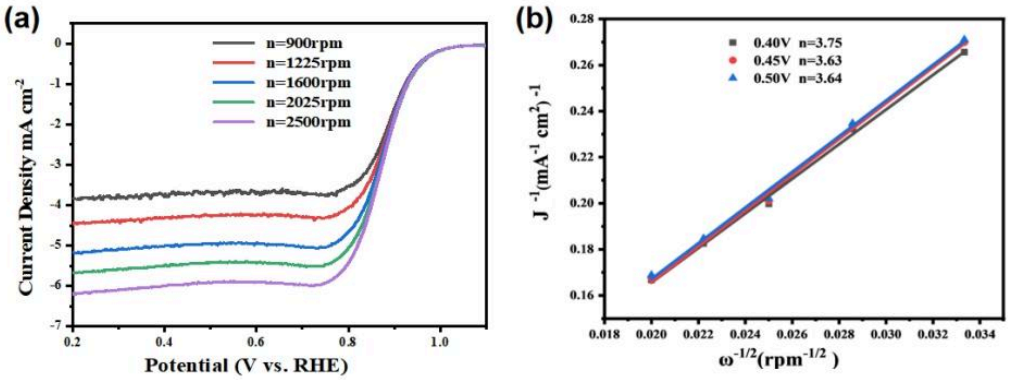


Figure 3. (a) Linear sweep voltammetry test of FeCo-NC in the speed range of 900–2500 rpm; (b) Koutecky-Levich (K-L) curve analysis to calculate the number of electron transfers n

To get even more insight into the catalytic kinetics of the ORR, we performed Tafel analysis based on the LSV curves obtained at 1600 rpm for the different catalysts, and the results are summarized in Figure 4. The Tafel slope—a key kinetic parameter derived from the relationship between overpotential and the log of current density—tells us a lot about the rate-determining step and the underlying reaction mechanism. When we compared the Tafel slopes of the different catalysts, we saw some clear differences. More specifically, the bimetallic FeCo-NC catalyst showed a Tafel slope of 96 mV dec^{-1}. That value is noticeably higher than what we got for the monometallic Co-NC variants, but it's still lower than that of the commercial Pt/C benchmark. This intermediate value suggests that FeCo-NC has favorable ORR kinetics, meaning it provides a more efficient catalytic interface for oxygen reduction than its single-atom counterparts. The enhanced kinetic behavior can be traced back to the synergistic interaction between the Fe and Co metal sites embedded in the nitrogen-doped carbon matrix, which helps optimize the electronic configuration and promotes better adsorption and desorption of oxygen intermediates. Even though the Tafel slope is still a bit higher than that of Pt/C, the bimetallic catalyst still beats traditional non-noble metal catalysts in terms of kinetic performance. It enables faster electron transfer and more efficient reactant conversion during the ORR process. These results really highlight how effective the

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bimetallic design strategy is for tuning electrocatalytic properties and improving overall reaction kinetics, and they point to FeCo-NC as a durable and highly active catalyst for advanced energy technologies.

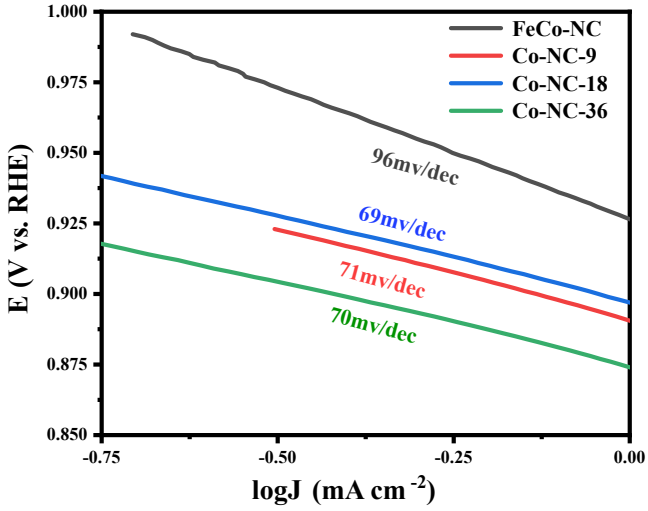


Figure 4. Tafel curves of different catalysts

4. Conclusion and outlook

In this study, we used ZIF-8/ZIF-67 as precursors and applied a solvent-thermal method together with high-temperature calcination of the ZIF material to successfully make Co-NC electrocatalysts [28]. The electrochemical test results we got indicated that the catalyst shows its best electrocatalytic performance when the zinc-to-cobalt molar ratio is 18:1. So, based on that precursor composition, we introduced an iron source before the high-temperature calcination step to prepare the FeCo-NC bimetallic catalyst. Our experimental results show that this bimetallic catalyst really does exhibit outstanding electrocatalytic activity, with a half-wave potential of 0.875 V, and that performance is comparable to what you get with commercial Pt/C catalysts [29]. That offers an innovative way to get past the technical bottlenecks that zinc-air batteries currently face. In addition, when we characterized the material using scanning electron microscopy (SEM), we confirmed that the metal active sites in the material are indeed atomically dispersed. This indirectly tells us that metal catalytic efficiency is at its best when you work at the atomic level. Compared to single-atom catalysts, bimetallic catalysts take advantage of the synergistic effects between the metal sites to achieve performance that's on par with noble metal benchmark materials [30], and on top of that, they have big cost advantages. That gives them enormous application potential in electrochemical reactions and broad prospects for industrialization. Based on the research we've done, we'd like to offer the following outlook:

(1) One thing to explore is more precise synthesis methods. Even though quite a few synthesis strategies for bimetallic catalysts have been reported, it's still pretty challenging to get the structural precision we would like. Given the broad industrial application prospects that bimetallic synergy offers, future research could potentially use artificial intelligence (AI) technology to help with the design and achieve more precise synthesis. For example, computational methods like density

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functional theory (DFT) or d-band center theory could be used to further predict and optimize those precise synthesis methods..

(2) Another point is that we need to do more in-depth mechanistic studies. Even though some research has been done on the reaction mechanisms of bimetallic catalysts in catalytic processes, this area is still in its early stages compared to the relatively well-established research framework for single-atom catalysts. Right now, our understanding of the intrinsic mechanisms behind bimetallic synergy, the structure-activity relationships, and the complex reaction mechanisms that operate under real conditions is still pretty limited [31]. Fundamental scientific questions—like how the bimetallic synergy actually works, what the coordination environment looks like, and how the metals interact with the support—still need further and deeper analysis..

(3) The third thing is that we need to systematically clarify the "structure-activity" relationship. Besides choosing which metal combinations to use, we also have to consider the coordination environment and the metal-support interactions. Going forward, it's essential to take multiple factors into account so we can systematically figure out the intrinsic connection between structural features and catalytic activity, and that will help us refine our mechanistic studies even further. This is really important for enhancing catalytic performance, and it could very well drive breakthrough progress in the application of bimetallic catalysts in the clean energy sector.

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