



## Adsorption

### 1-An Adsorption Model Considering Fictitious Stress

By [Tan, XH](#) (Tan, Xiaohua) [\[1\]](#) ; [Ma, XJ](#) (Ma, Xinjian) [\[1\]](#) ; [Li, XP](#) (Li, Xiaoping) [\[1\]](#) ; [Li, YL](#) (Li, Yilong) [\[1\]](#) (provided by Clarivate) Source [FRACTAL AND FRACTIONAL](#) Volume 9 Issue 1 DOI

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Document Type Article

#### Abstract

The adsorption of coalbed methane alters the pore structure of reservoirs, subsequently affecting the coal seam's gas adsorption capacity. However, traditional gas adsorption models often neglect this crucial aspect. In this article, we introduce a fractal capillary bundle model that accounts for the expansion of coal seam adsorption. We utilize curvature fractal dimension and capillary fractal dimension to characterize the complexity of the coal seam's pore structure. By incorporating the concept of fictitious stress, we have described the relationship between gas adsorption, matrix porosity, and permeability changes. We have developed a model that describes the changes in matrix porosity and permeability during the gas adsorption process. After fitting this model to experimental data, it demonstrated high accuracy in predictions. Furthermore, our investigation into how factors such as curvature fractal dimension, capillary fractal dimension, and fictitious stress influence gas adsorption capacity reveals several key findings. Firstly, the specific surface area within the pore structure of coal seams is the primary factor controlling gas adsorption capacity. Secondly, the virtual stress generated during the gas adsorption process alters the coal seam's maximum gas adsorption capacity, a factor that cannot be overlooked. Lastly, we found that gas adsorption primarily affects the gas migration process, while under high-pressure conditions, gas desorption does not cause significant changes in the matrix porosity and permeability.

#### Keywords

#### Author Keywords

[coal](#)[coal adsorption capacity](#)[adsorption model](#)[fractal approach](#)[fictitious stress](#)

#### Keywords Plus

[PORE STRUCTURE](#)[CH4 ADSORPTION](#)[FRACTAL CHARACTERIZATION](#)[METHANE ADSORPTION](#)[PERMEABILITY MODEL](#)[GAS-ADSORPTION](#)[CAPACITY](#)[PARTICLE](#)[EQUATION](#)[COALS](#)

## Adsorption

### 2-Advancements in CO2 capture by absorption and adsorption: A comprehensive review

By Soo, XYD (Soo, Xiang Yun Debbie) [1] ; Lee, JJC (Lee, Johnathan Joo Cheng) [1] ; Wu, WY (Wu, Wen-Ya) [1] ; Tao, LG (Tao, Longgang) [2] ; Wang, C (Wang, Cun) [2] ; Zhu, Q (Zhu, Qiang) [1] , [2] , [3] ; Bu, J (Bu, Jie) [2] (provided by Clarivate) Source JOURNAL OF CO2 UTILIZATION Volume 81 DOI 10.1016/j.jcou.2024.102727 Article Number 102727 Published MAR 2024 Early Access MAR 2024  
Indexed 2024-05-31 Document Type Review

#### Abstract

In the face of escalating global climate challenges, effective carbon dioxide (CO<sub>2</sub>) capture techniques remain at the forefront of mitigating anthropogenic greenhouse gas emissions. This comprehensive review elucidates the latest advancements in CO<sub>2</sub> capture, emphasizing two predominant methodologies: absorption and adsorption. We delve into the mechanisms underlying each process, highlighting the novel materials and technologies that have emerged over recent years. For absorption, the focus is placed on the material design strategy, and identifying new materials in the class of amines, ionic liquids (ILs) and nanofluids for enhanced CO<sub>2</sub> capture capacities and reduced energy requirements. In the realm of adsorption, the synthesis of innovative adsorbents, such as metal organic framework (MOF), organic polymers, inorganic adsorbents, silicon-based adsorbents, and biochar and byproducts from biomass with superior selectivity and stability, is explored. Additionally, the review addresses the challenges associated with each method, offering insights into potential avenues for further research. By providing a holistic overview of the current landscape of CO<sub>2</sub> capture, this article serves as a pivotal resource for researchers and industry professionals aiming to advance sustainable solutions to combat climate change.

#### Keywords

#### Author Keywords

[Carbon dioxide capture](#)[Absorption](#)[Adsorption](#)[Chemical absorption](#)[Physical absorption](#)[Porous materials](#)[Carbon capture and storage](#)[Climate change mitigation](#)

#### Keywords Plus

[CARBON-DIOXIDE CAPTURE](#)[AMINE-BASED ABSORBENTS](#)[IONIC LIQUIDS](#)[QUEOUS-SOLUTIONS](#)[MASS-TRANSFER](#)[BIPHASIC SOLVENTS](#)[SLOW-VISCOSITY](#)[COMBUSTION TECHNOLOGY](#)[FE304](#)[NANOPARTICLES](#)[DIETHANOLAMINE](#)[DEA](#)



## Adsorption

### 3-Harnessing nitrogen doped magnetic biochar for efficient antibiotic adsorption and degradation

By Rana, P (Rana, Parul) [1] ; Soni, V (Soni, Vatika) [1] ; Sharma, S (Sharma, Simran) [1] ; Poonia, K (Poonia, Komal) [1] ; Patial, S (Patial, Shilpa) [2] ; Singh, P (Singh, Pardeep) [1] ; Selvasembian, R (Selvasembian, Rangabhashiyam) [4] ; Chaudhary, V (Chaudhary, Vishal) [3] ; Hussain, CM (Hussain, Chaudhery Mustansar) [5] ; Raizada, P (Raizada, Pankaj) [1] (provided by Clarivate) Source JOURNAL OF INDUSTRIAL AND ENGINEERING CHEMISTRY Volume 148 Page 174-195 DOI 10.1016/j.jiec.2025.01.025 Published AUG 25 2025 Early Access MAY 2025 Indexed 2025-06-13 Document Type Review

#### Abstract

Nitrogen-doped magnetic biochar (N-doped magnetic BC) has garnered significant attention as a multifunctional material for the remediation of antibiotic-contaminated water, owing to its synergistic adsorption and degradation capabilities. This review critically evaluates the transformative role of pretreatment strategies physicochemical attributes of biochar, focusing on nitrogen doping and chemical activation. These methodologies are complemented by post-treatment processes designed to impart synergistically optimized properties to the biochar matrix. Such modifications are pivotal in fine-tuning the material's characteristics, including surface area, pore architecture, and active site configuration, thereby enhancing its adsorption efficiency and catalytic performance. Advanced characterization techniques, such as electron microscopy, diffraction, and various spectroscopic modalities, provide comprehensive insights into the structural, and magnetic properties of nitrogen-doped magnetic BC. The adsorption mechanisms are predominantly driven by *it-it* interactions, hydrogen bonding, and electrostatic forces, with nitrogen doping and functionalization significantly amplifying the material's selectivity and adsorption capacity. Furthermore, catalytic degradation of antibiotics occurs via both radical and non-radical pathways, underscoring functionality of the material. Notably, N-doped magnetic BC demonstrates excellent recyclability, maintaining high efficiency across multiple adsorption-desorption cycles. This highlights its potential for sustainable cation. Future research directions proposed in this study emphasize advancing the eco-compatibility ability of N-doped magnetic BC. Computational modelling is suggested to predict and optimize the material's physicochemical properties, alongside the development of large-scale, environmentally benign synthesis techniques. These advancements aim to position N-doped magnetic BC as a cornerstone material in wastewater treatment systems.

#### Keywords

#### Author Keywords

[N-Doped biochar](#)[Magnetic biochar](#)[Antibiotic removal](#)[Adsorption](#)[Catalytic degradation](#)[Mechanistic insights](#)

#### Keywords Plus

[WATER-TREATMENT](#)[AQUATIC ENVIRONMENT](#)[REMOVAL](#)[PERSULFATE](#)[RESOURCES](#)[OXIDATION](#)



## Adsorption

### 4-Adsorption-attraction electrolyte addressing anion-deficient interface for lithium metal batteries

By Lai, PB (Lai, Pengbin) [1] ; Zhang, YQ (Zhang, Yaqi) [1] ; Wang, JH (Wang, Junhao) [1] ; Chen, MH (Chen, Minghui) [1] ; Li, XY (Li, Xinyu) [2] ; Deng, XD (Deng, Xiaodie) [1] ; Chen, QC (Chen, Qichen) [2] ; Huang, BY (Huang, Boyang) [1] ; Gan, CL (Gan, Chaolun) [3] ; Zou, YG (Zou, Yeguo) [1] ; (provided by Clarivate) Source ESCIENCE Volume 5 Issue 5 DOI 10.1016/j.esci.2025.100399

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Document Type Article

#### Abstract

Constructing an optimal solid-electrolyte interphase (SEI) through electrolyte strategies is an effective approach to suppress lithium dendrites and improve deposition/stripping reversibility. Specifically, increasing the proportion of anion coordination in the inner Li<sup>+</sup> solvation sheath promotes the formation of an anion-derived SEI that features a high content of inorganic components favoring Li<sup>+</sup> diffusion. However, whether this anion-rich structure can persist during cycling has not been dynamically investigated. In this work, we not only construct a favorable solvation structure but also study its evolution in both bulk and interface regions across varying temperatures. Additionally, we employ the unique "adsorption-attraction" mechanism of trifluoromethoxybenzene (PhOCF<sub>3</sub>) solvent to inhibit the undesirable transition from an "anion-rich" to "anion- deficient" structure at the anode interface, which is confirmed by 2D NMR and *in situ* infrared spectroscopy. In summary, this work explores the solvation structure in depth and proposes new perspectives on designing electrolytes for lithium metal batteries.

#### Keywords

#### Author Keywords

Solvation structureIn situ characterizationLithium metal batteryLow temperatureLocalized high-concentration electrolyte

#### Keywords Plus

HIGH-ENERGY ANODESLi<sup>+</sup>



## Adsorption

### 5-Innovations and challenges in adsorption-based wastewater remediation: A comprehensive review

By Satyam, S (Satyam, Satyam) [1] ; Patra, S (Patra, Sanjukta) [1] (provided by Clarivate)

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#### Abstract

Water contamination is an escalating emergency confronting communities worldwide. While traditional adsorbents have laid the groundwork for effective water purification, their selectivity, capacity, and sustainability limitations have driven the search for more advanced solutions. Despite many technological advancements, economic, environmental, and regulatory hurdles challenge the practical application of advanced adsorption techniques in large-scale water treatment. Integrating nanotechnology, advanced material fabrication techniques, and datadriven design enabled by artificial intelligence (AI) and machine learning (ML) have led to a new generation of optimized, high-performance adsorbents. These advanced materials leverage properties like high surface area, tailored pore structures, and functionalized surfaces to capture diverse water contaminants efficiently. With a focus on sustainability and effectiveness, this review highlights the transformative potential of these advanced materials in setting new benchmarks for water purification technologies. This article delivers an in-depth exploration of the current landscape and future directions of adsorbent technology for water remediation, advocating for a multidisciplinary approach to overcome existing barriers in large-scale water treatment applications.

#### Keywords

##### Author Keywords

[Wastewater remediation](#)[Adsorbent materials](#)[Water purification](#)[Material science](#)[Nanotechnology](#)[Metal organic framework](#)[Advanced fabrication methods](#)[Artificial intelligence](#)[Machine learning](#)[Sustainable solutions](#)

##### Keywords Plus

[COVALENT ORGANIC FRAMEWORK](#)[ENHANCED ADSORPTION](#)[METHYL-ORANGE](#)[FORCE-FIELD](#)[REMOVAL](#)[ADSORBENTS](#)[BIOCHAR](#)[DEGRADATION](#)[SULFAMETHOXAZOLE](#)[NANOMATERIALS](#)



## Adsorption

## 6-The Weber-Morris model in water contaminant adsorption: Shattering long-standing misconceptions

By Chu, KH (Chu, Khim Hoong) [1] , [2] ; Hashim, MA (Hashim, Mohd Ali) [2] ; Zawawi, MH (Zawawi, Mohd Hafiz) [1] , [3] ; Bollinger, JC (Bollinger, Jean-Claude) [4] (provided by Clarivate) Source JOURNAL OF ENVIRONMENTAL CHEMICAL ENGINEERING Volume 13 Issue 4 DOI 10.1016/j.jece.2025.117266 Article Number 117266 Published AUG 2025 Early Access MAY 2025 Indexed 2025-06-14 Document Type Article

## Abstract

The Weber-Morris (W-M) intraparticle diffusion model is widely used to analyze the kinetics of water contaminant adsorption. However, this article shows that the model has been routinely misapplied and misinterpreted in recent studies. We critically examine three prevalent but unfounded claims associated with the W-M model: (1) a linear plot that does not pass through the origin indicates that intraparticle diffusion is not the dominant mechanism; (2) the intercept, which may be positive or negative, represents boundary layer thickness; and (3) multiple linear segments correspond to distinct mass transport processes. Our analysis shows that these claims arise from a misrepresentation of the original W-M model, one lacking theoretical support and rendering such interpretations invalid. While the original W-M model can be useful when applied correctly, it is inherently limited to the initial phase of adsorption, as it approximates the exact infinite series solution to an intraparticle diffusion model. For more rigorous and comprehensive kinetic analyses, we recommend adopting more robust alternatives, such as the Vermeulen and Helfferich-Plesset approximations, which are valid across the full adsorption profile. Ideally, the exact infinite series solution should be used, as it can now be readily implemented using modern computational tools.

## Keywords

## Author Keywords

## Homogeneous solid diffusionPore and surface diffusionSquare root of time plotHelfferich and PlessetReichenbergVermeulen

## Keywords Plus

## INTRAPARTICLE DIFFUSION KINETICS COEFFICIENTS ADSORBENT SSORPTION REMOVAL COLOR BATCH

## Adsorption

### 7-Optimization of Adsorption Sites for Selective Hydrobenzoin and Syngas Production in a Single Photoredox Cycle

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By Lei, J (Lei, Jian) [1] ; Yang, HY (Yang, Hongyuan) [4] ; Weng, B (Weng, Bo) [2] , [3] ; Zheng, YM (Zheng, Yu-Ming) [2] , [3] ; Chen, SF (Chen, Shifu) [6] ; Menezes, PW (Menezes, Prashanth W.) [4] , [5] ; Meng, SG (Meng, Sugang) [1] , [6] (provided by Clarivate) Source ADVANCED ENERGY MATERIALS Volume 15 Issue 29 DOI 10.1002/aenm.202500950 Published AUG 2025 Early Access MAY 2025 Indexed 2025-05-10 Document Type Article

#### Abstract

Integrating benzyl alcohol oxidation with carbon dioxide (CO<sub>2</sub>) reduction in a single photoredox catalysis is of high economic and practical interest. However, it remains challenging to controllably regulate the selectivity of specific C & horbar;C coupling chemicals (oxidation products) and the ratio of carbon monoxide and hydrogen (CO/H<sub>2</sub>) for syngas (reduction products). Herein, an efficient photocatalyst consisting of CdS nanorods decorated by Ni<sub>2</sub>P (NP/CdS) is developed, which achieves remarkable performance, producing C & horbar;C coupling hydrobenzoin (HB) with an excellent yield of approximate to 315.4  $\mu\text{mol g}^{-1}\text{h}^{-1}$  and selectivity of approximate to 90%. This performance originates from the optimized adsorption of benzaldehydes and protons, promoting the generation of the critical radical intermediates (center dot CH(OH)Ph). Meanwhile, the favorable desorption of center dot CH(OH)Ph and HB from the binding sites is attained. On the other hand, by increasing the Ni<sub>2</sub>P content in NP/CdS, the CO/H<sub>2</sub> ratio can be adjusted across a wide range (from approximate to 15:1 to approximate to 2.6:1), enabling syngas compositions suitable for industrial feedstock applications. This tunability is attributed to the lower CO<sub>2</sub> affinity of the Ni<sub>2</sub>P phase compared to CdS while demonstrating higher activity for H<sub>2</sub> evolution. This work presents a novel approach for selectively and efficiently producing HB and tunable syngas simultaneously.

#### Keywords

#### Author Keywords

[adsorption site manipulation](#)[benzyl alcohol oxidation](#)[carbon dioxide reduction](#)[hydrobenzoin](#)[photoredox catalysis](#)[in situ](#)[tunable syngas](#)



## Adsorption

### 8-Constructing multiple sites porous organic polymers for highly efficient and reversible adsorption of triiodide ion from water

By Li, ZY (Li, Zhiyong) [1] ; Fu, YB (Fu, Yibo) [1] ; Li, YL (Li, Yilong) [1] ; Li, RP (Li, Ruipeng) [1] ; Pei, YC (Pei, Yuanchao) [1] ; Shi, YL (Shi, Yunlei) [1] ; Wang, HY (Wang, Huiyong) [1] (provided by Clarivate)

Source GREEN ENERGY & ENVIRONMENT Volume 10 Issue 8 DOI 10.1016/j.gee.2025.03.005

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#### Abstract

The utilization of nuclear power will persist as a prominent energy source in the foreseeable future. However, it presents substantial challenges concerning waste disposal and the potential emission of untreated radioactive substances, such as radioactive I-129 and I-131. The transportation of radioactive iodine poses a significant threat to both the environment and human health. Nevertheless, effectively, rapidly removing iodine ion from water using porous adsorbents remains a crucial challenge. In this work, three kinds of multiple sites porous organic polymers (POPs, POP-1, POP-2, and POP-3) have been developed using a monomer pre-modification strategy for highly efficient and fast I-3(-) absorption from water. It is found that the POPs exhibited exceptional performance in terms of I-3(-) adsorption, achieving a top-performing adsorption capacity of 5.25 g g(-1) and the fastest average adsorption rate ( $K_{80}(\%) = 4.25 \text{ g g}(-1) \text{ h}(-1)$ ) with POP-1. Moreover, POP-1 exhibited exceptional capacity for the removal of I-3(-) from flowing aqueous solutions, with 95% removal efficiency observed even at 0.0005 mol L<sup>-1</sup>. Such results indicate that this material has the potential to be utilized for the emergency preparation of potable water in areas contaminated with radioactive iodine. The adsorption process can be effectively characterized by the Freundlich model and the pseudo-second-order model. The exceptional I-3(-) absorption capacity is primarily attributed to the incorporation of a substantial number of active adsorption sites, including bromine, carbonyl, and amide groups. (c) 2025 Institute of Process Engineering, Chinese Academy of Sciences. Publishing services by Elsevier B.V. on behalf of KeAi Communications Co., Ltd. This is an open access article under the CC BY-NC-ND license (<http://creativecommons.org/licenses/by-nc-nd/4.0/>).

#### Keywords

#### Author Keywords

[Triiodide ion](#)[Porous organic polymer](#)[Efficient adsorption](#)[Multiple site](#)[Interaction](#)

#### Keywords Plus

[IODINE CAPTURE](#)[FRAMEWORKS](#)[AEROGELS](#)[REMOVAL](#)[NANOCOMPOSITE](#)[EMISSIONS](#)[CHERNOBYL](#)[ZEOLITES](#)[129](#)



## Adsorption

### 9-Boosting $\text{NH}_4^+$ adsorption of $\text{Ti}_3\text{C}_2\text{T}_x@\text{S-V}_2\text{O}_5@\text{CNF}$ nanofiber by S doping and heterostructure construction: local charge regulation

By Wang, HY (Wang, Hai-Yang) [1] ; Luo, H (Luo, Hao) [1] ; Liang, MM (Liang, Miao-Miao) [2] ; Ma, H (Ma, Hao) [1] ; Lv, D (Lv, Du) [1] ; Qu, F (Qu, Fan) [1] ; Yin, Y (Yin, Ying) [3] ; Zhou, Y (Zhou, Yuan) [4] ; Zhang, XD (Zhang, Xu-Dong) [5] ; Zhao, HC (Zhao, Hai-Chao) [6] ; (provided by Clarivate) Source RARE METALS Volume 44 Issue 7 Page 4642-4656 DOI 10.1007/s12598-025-03325-8 Published JUL 2025 Early Access MAY 2025 Indexed 2025-05-28 Document Type Article

#### Abstract

Aqueous ammonium ion battery (AAIB) is considered as a promising candidate for next-generation energy storage device, while the limited performance of cathode material retards its further development. Seeking novel materials and reveal the underlying energy storage reinforcement mechanism is necessary for promoting future commercial application of AAIB. Herein, a novel electrospun  $\text{Ti}_3\text{C}_2\text{T}_x@\text{S-V}_2\text{O}_5@\text{CNF}$  nanofiber is constructed by sulfur doping and  $\text{Ti}_3\text{C}_2\text{T}_x$  introduction strategy to exert the synergetic effect on  $\text{NH}_4^+$  storage capacity. Density functional theory calculations indicate that the induction of  $\text{Ti}_3\text{C}_2\text{T}_x$  can redistribute the internal charges of material, induce the downshift of the d-band center of V atoms and p-band center of S atoms to the Fermi level, thus the adsorption energy of  $\text{NH}_4^+$  is optimized. Electrochemical results show that the  $\text{Ti}_3\text{C}_2\text{T}_x@\text{S-V}_2\text{O}_5@\text{CNF}$  electrode displays high capacity of 576.2 mAh g<sup>-1</sup> at 0.5 A g<sup>-1</sup>, long cycle life and superior rate performance. The assembled  $\text{Ti}_3\text{C}_2\text{T}_x@\text{S-V}_2\text{O}_5@\text{CNF//PTCDI}$  full cell also exhibits excellent electrochemical behavior including large specific capacity of 181 mAh g<sup>-1</sup> at 0.5 A g<sup>-1</sup>, cycling stability of 10,000 cycles at 5 A g<sup>-1</sup> with no capacity decay, and good rate performance. This work gives insight into the  $\text{NH}_4^+$  storage capacity control by rational local charge regulation through S doping and heterostructure construction to facilitate electron transfer for AAIBs and other energy storage system.

#### Keywords

#### Author Keywords

[Aqueous ammonium ion battery](#) [\$\text{Ti}\_3\text{C}\_2\text{T}\_x@\text{S-V}\_2\text{O}\_5@\text{CNF}\$](#) [Charge regulation](#)



## Adsorption

### 10-Coupled effects of the anisotropic permeability and adsorption-induced deformation on the hydrogen and carbon reservoir extraction dynamics

By Wang, LC (Wang, Linchao) [1] ; Zhang, W (Zhang, Wan) [1] ; Cao, ZZ (Cao, Zhengzheng) [2] ; Xue, Y (Xue, Yi) [1] ; Xiong, F (Xiong, Fei) [3] (provided by Clarivate) Source PHYSICS OF FLUIDS

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#### Abstract

Hydrogen and carbon energy reservoirs, critical resources for clean energy development, require precise characterization of their mechanical and fluid flow properties. This study investigates the coupled effects of anisotropic permeability and adsorption-induced deformation on gas extraction efficiency in such reservoirs. A comprehensive numerical model is developed to integrate matrix deformation, crack anisotropy, and adsorption-driven anisotropic swelling within coal reservoirs. The model extends the Langmuir isotherm to incorporate directional adsorption effects and employs a strain-ratio mechanism to quantify permeability evolution induced by non-uniform stresses. Finite element simulations reveal that declining gas pressure near the wellbore intensifies permeability gradients. This finding underscores the necessity of accounting for adsorption-induced volumetric strain to prevent overestimation of coal permeability in traditional models. Anisotropic stress confinement significantly affects gas extraction dynamics, with horizontal permeability ( $k_x$ ) increasing more gradually under depletion compared to vertical permeability ( $k_y$ ). The results highlight pronounced directional variations in extraction rates, with  $x$ -direction rates reaching only half of those in the  $y$  direction. These findings underscore the importance of addressing permeability anisotropy and adsorption effects to optimize reservoir performance. The study offers valuable insights into the sustainable development of hydrogen and carbon energy resources, providing a theoretical foundation for enhancing gas recovery strategies.

#### Keywords

#### Keywords Plus

[GAS-FLOW](#)[COALBED](#) [METHANE](#)[MODEL](#)[EVOLUTION](#)[DRAINAGE](#)[SORPTION](#)[CO2](#)



## Adsorption

### 11-Strong coupling Fe<sub>2</sub>VO<sub>4</sub> nanoparticles/3D N-doped interconnected porous carbon derived from MOFs by confined adsorption-assembly-pyrolysis for greatly boosting oxygen reduction

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By Liu, LL (Liu, Ling-Ling) [1] ; Liu, L (Liu, Lu) [1] , [2] ; Wang, CY (Wang, Chen-Yang) [1] ; Zhang, L (Zhang, Lu) [1] ; Feng, JJ (Feng, Jiu-Ju) [1] ; Gao, YJ (Gao, Yi-Jing) [1] , [2] ; Wang, AJ (Wang, Ai-Jun) [1] (provided by Clarivate) Source JOURNAL OF COLLOID AND INTERFACE SCIENCE Volume 684 Page 10-20 Part 2 DOI 10.1016/j.jcis.2025.01.052 Published APR 15 2025 Early Access JAN 2025 Indexed 2025-02-21 Document Type Article

#### Abstract

Low-cost and effective electrocatalysts are critical for energy storage and conversion. Herein, iron(III) and vanadium(III) acetylacetones were first adsorbed and confined in porous zeolitic imidazolate framework-8 (ZIF8), which further cross-linked together by the methanol-induced-assembly. Following the pyrolysis, the Fe<sub>2</sub>VO<sub>4</sub> nanoparticles were efficiently encapsulated within three-dimensional (3D) N-doped interconnected porous carbon, termed Fe<sub>2</sub>VO<sub>4</sub>/NIPC. The obtained Fe<sub>2</sub>VO<sub>4</sub>/NIPC displayed outstanding catalytic properties in the alkaline media for oxygen reduction reaction with a half-wave potential of 0.86 V. In the parallel, density functional theory (DFT) calculations were performed to illustrate the catalytic mechanism. Moreover, the Fe<sub>2</sub>VO<sub>4</sub>/NIPC assembled Zn-air battery showed a high peak power density of 107.7 mW cm<sup>-2</sup> and excellent long-cycle stability over a duration of 250 h, which outperformed commercial Pt/C catalyst in the control group. The strong coupling and synergistic effects between the Fe<sub>2</sub>VO<sub>4</sub> nanoparticles and N-doped carbon improved the catalytic performance, coupled by promoting the stability. This study opens a prospect way to develop high-efficiency carbon-based electrocatalysts in energy storage and conversion devices.

#### Keywords

#### Author Keywords

[Confined adsorption](#)[Pyrolysis](#)[Oxygen reduction reaction](#)[Transition metal oxides](#)[Zinc-air batteries](#)

#### Keywords Plus

[IRONELECTROCATALYSTSFECO](#)