

## PERSPECTIVE

# Advancing porous materials for radioiodine capture

To cite this article: Qiuyu Rong *et al* 2025 *Nanotechnology* **36** 252501

View the [article online](#) for updates and enhancements.

## You may also like

- [Retention and endurance analysis for 2T0C DRAM based on ALD-ITZO thin film transistors](#)  
Jingxuan Wei, Yu Zhang, Nannan Li et al.
- [Hybrid-contact engineering for enhanced p-type performance in WSe<sub>2</sub> field-effect transistors](#)  
Zhe Chen, Lanxin Xu, Yingjie Zhao et al.
- [High energy density symmetric supercapacitors coupling redox-active gel polymer electrolytes with N-doped carbons](#)  
Undavalli Venkata Gopi, Akash Sai S M and Kumar Sai Smaran



## Perspective

# Advancing porous materials for radioiodine capture

Qiuyu Rong<sup>1</sup>, Mengjie Hao<sup>1</sup>,  
Zhongshan Chen<sup>1</sup>, Hui Yang<sup>1,\*</sup>,  
Geoffrey I N Waterhouse<sup>2</sup> ,  
Shengqian Ma<sup>3</sup>  
and Xiangke Wang<sup>1,\*</sup>

<sup>1</sup> College of Environmental Science  
and Engineering, North China

Electric Power University, Beijing  
102206, People's Republic of China

<sup>2</sup> School of Chemical Sciences, The  
University of Auckland, Auckland  
1142, New Zealand

<sup>3</sup> Department of Chemistry,  
University of North Texas, Denton,  
TX 76201, United States of America  
E-mail: [h.yang@ncepu.edu.cn](mailto:h.yang@ncepu.edu.cn)  
and [xkwang@ncepu.edu.cn](mailto:xkwang@ncepu.edu.cn)

## Abstract

Radioactive iodine, released during nuclear accidents and spent fuel treatment, poses significant threats to ecosystems and human health due to its volatility, persistence, and potential for bioaccumulation. Porous materials with tunable structures and tailored adsorption sites have recently emerged as a promising technology for iodine capture. This paper reviews the progress of research on porous materials for iodine capture, focusing on improvements in iodine capture performance as well as adsorbent stability through innovative structure–function strategies. Finally, we propose innovative directions for future research, including the design of multifunctional composite materials, integration of electrochemical and photocatalytic technologies, and leveraging machine learning for material optimization and performance prediction. These approaches offer new pathways to enhance iodine capture efficiency and advance nuclear safety through more effective radionuclide management approaches.

**Keywords:** porous materials, radioactive iodine, capture, covalent organic frameworks, porous organic cages

## 1. Introduction

Radioactive iodine (<sup>129</sup>I and <sup>131</sup>I) primarily originates from nuclear fission reaction [1]. <sup>129</sup>I has a long half-life ( $15.7 \times 10^7$  years) and significant environmental persistence, while <sup>131</sup>I, with a shorter half-life (8 d), is highly biologically active and can accumulate in the thyroid, creating health risks [1, 2]. Both pose ongoing threats to human health and ecosystems if not adequately contained. During the operation of nuclear power plants, nuclear weapons testing, and spent fuel reprocessing, radioactive iodine can exist in the gas phase (I<sub>2</sub>, CH<sub>3</sub>I) and liquid phase (I<sup>−</sup>, IO<sub>3</sub><sup>−</sup>) [3]. Therefore, the implementation of effective measures to capture and contain these different forms of radioactive iodine is essential.

The capture principles of iodine and radioactive iodine are fundamentally similar, relying on physical adsorption, chemical adsorption, and chemical reactions. Iodine capture methods include physical adsorption [4], chemical adsorption [5], ion exchange [3], and complexation [6], etc. Porous materials exhibit different gaseous and liquid-phase iodine capture mechanisms, depending on their pore structure, surface chemistry, and iodine's physicochemical state. For gaseous iodine removal, physical and chemical adsorption methods dominate. Pore design plays a crucial role in physical adsorption, leveraging high surface area and abundant porosity. Notably, micropores (<2 nm) are critical, as their size closely matches iodine's van der Waals radius (~4.5 Å), enabling exploitation of van der Waals interactions that enhance the adsorption capacity. Chemical adsorption involves several mechanisms: (i) electron-rich functional groups (e.g.

\* Authors to whom any correspondence should be addressed.

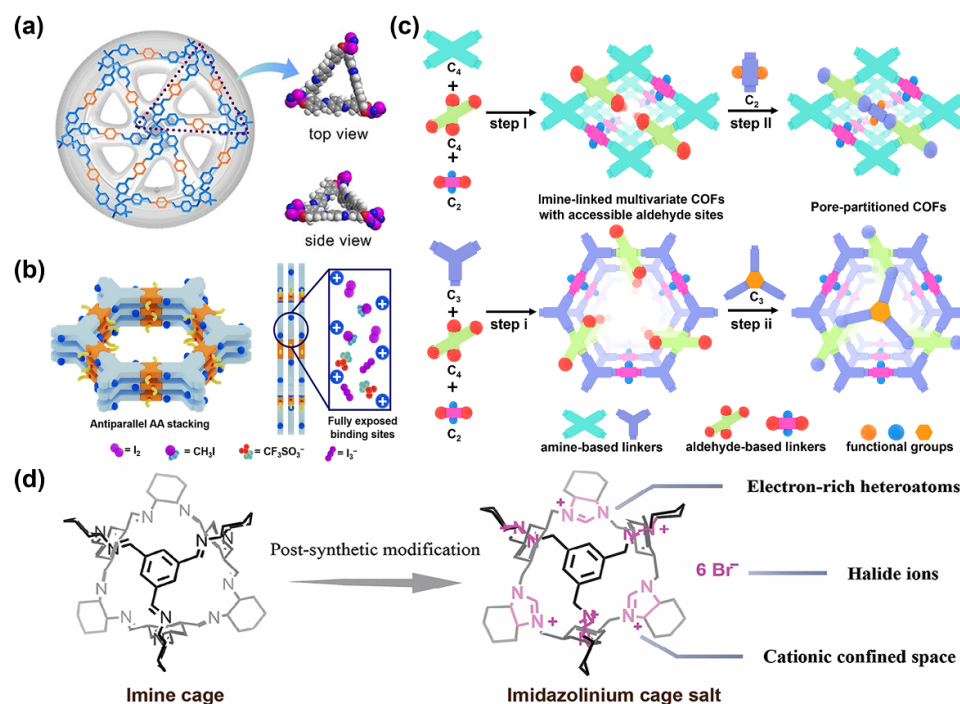
aromatic rings, nitrogen heterocycles) facilitate adsorption via  $\pi$ - $\pi$  interactions or charge transfer effects [7, 8]; (ii) nitrogen-containing sites (e.g. imidazole, triazine, pyridine) enhance  $I_2/I_3^-$  capture through hydrogen bonding or electrostatic interactions [8, 9]; (iii) active sites such as unsaturated metal oxides centers provide additional adsorption energy and reactivity [10], improving iodine fixation. Besides physical adsorption, ion exchange and complexation play key roles in liquid-phase systems. Porous materials with exchangeable ions (e.g.  $Cl^-$ ) can capture iodine via ion exchange, while specific metal ions, such as  $Ag^+$ , react with  $I^-$  to form insoluble  $AgI$  precipitates, ensuring effective iodine sequestration. Besides, radioactive iodine capture emphasizes irreversible fixation, long-term stability, secondary pollution release prevention, and geological sequestration. This is typically achieved using chemically stable materials or immobilization methods like vitrification [11] and ceramic doping [12].

However, research on the capture of iodine still faces several challenges, including: (i) low capture efficiency of traditional adsorbents; (ii) inadequate adsorbent stability under extreme conditions (e.g. high temperature, high humidity, and radiation exposure); (iii) low  $CH_3I$  concentrations and weak intermolecular forces; (iv) scalability and cost-effectiveness. Therefore, the development of efficient and stable adsorbent materials for radioiodine in its various forms is of significant practical importance.

In recent years, significant progress has been made in the capture of gas-phase and aqueous iodine. Porous materials (e.g. covalent organic frameworks (COFs) [13, 14], porous organic polymers (POPs) [15], porous organic cages (POCs) [16], metal-organic frameworks (MOFs) [17, 18], and certain inorganic porous materials [19–21] have notably enhanced the field of iodine capture due to their exceptional adsorption capacity, excellent structural designability, and broad potential for functionalization to allow selective capture of iodine species. Various innovative strategies in material design and optimization have been introduced to address the challenges faced in iodine capture.

## 2. Application of porous materials in iodine capture

To address issues of low iodine capture efficiency and material instability, Guo *et al* [22] first reported that a string of 2D COFs with quasi-three-dimensional (QTD) topologies and coliform-like crystalline forms. These materials possess inimitable ‘stereoscopic’ trilateral pores, flexible construction blocks, and large interlayer spacings (figure 1(a)), which enable QTD-COFs to exhibit faster iodine adsorption rates than traditional 2D COFs. QTD-COF-V achieves an adsorption capacity of  $6.29\text{ g g}^{-1}$  ( $75\text{ }^\circ\text{C}$ , 1 bar), and maintains  $6.02\text{ g g}^{-1}$  after irradiation, demonstrating its potential for radioactive iodine capture under real-world conditions. Furthermore, the study elucidates the iodine capture mechanism and transport pathways through Raman spectroscopy, FT-IR, and XPS analyses. Iodine molecules can simultaneously enter the Q-3D channels of the material through both the top and lateral surfaces, interacting with the electron-rich conjugated system to form  $I_5^-$  charge-transfer complexes. The flexible framework of the QTD-COFs can adaptively adjust the pore size to facilitate iodine diffusion. Ultimately, the synergistic effects of physical confinement and chemical bonding enable the stable immobilization of iodine, significantly enhancing the adsorption rate and capacity of iodine. By introducing N-sites into the structure, the affinity for both  $I_2$  and  $CH_3I$  can be greatly enhanced. Xie *et al* [9] developed ACOF-1, featuring an anti-parallel AA stacking structure (figure 1(b)) and excellent radiation resistance. Pyridine-N and hydrazine units in the pores enable dynamic adsorption capacities of  $CH_3I$  for  $\sim 0.74\text{ g g}^{-1}$  and  $I_2$  for  $\sim 2.16\text{ g g}^{-1}$  at  $25\text{ }^\circ\text{C}$ . Additionally, the methylated cationic framework ACOF-1 R purifies iodine-contaminated groundwater to potable levels rapidly,



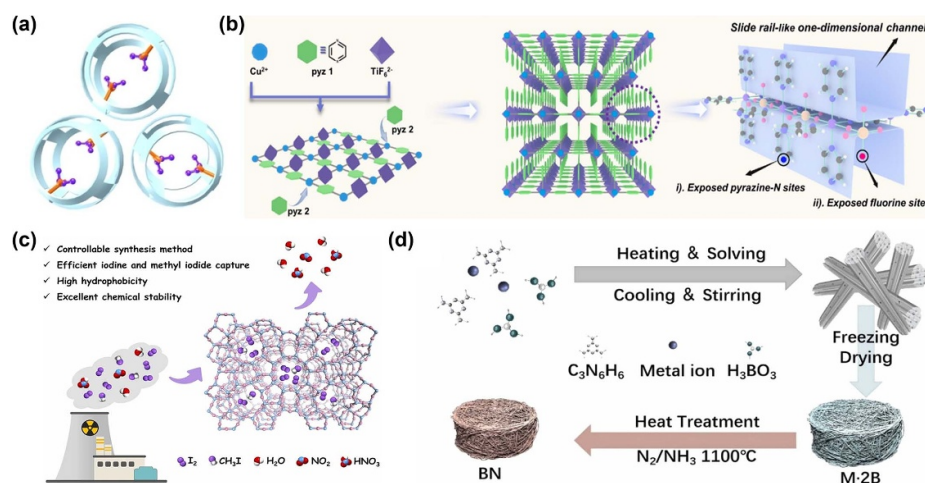
**Figure 1.** (a) The unique oblique triangular pores of QTD-COFs. [22] John Wiley & Sons.© 2020 Wiley-VCH GmbH. (b) Schematic illustration of anti-parallel AA stacking in COF-based adsorbents, showing how antiparallel stacked layers form three-dimensional ‘multi-N nanotraps’ for iodine species, significantly enhancing the utilization and affinity of chelating sites Adapted from [9]. CC BY 4.0. (c) Illustration of the pore partition synthetic strategy in imine-linked multivariate COFs, showing the synthesis of multicomponent COFs with predesigned accessible aldehyde sites, followed by the introduction of a symmetric building block as the pore partition agents to divide one micropore/mesopore into two or three micropores Reprinted (adapted) with permission from [23]. Copyright (2024) American Chemical Society. (d) Enhancing the  $I_2$  affinity of the porous organic cage through post-synthetic modification. Adapted from [25]. CC BY 4.0.

with a high adsorption rate of up to  $\sim 4.46 \text{ g g}^{-1}$  for  $I_3^-$ , offering valuable insights for triiodide removal from wastewater. The pyridine-N sites and interlayer hydrazine groups in the material form ‘multi-N nanotrap sites,’ which synergistically and effectively adsorb  $I_2$  and  $CH_3I$ . Subsequently, a post-synthetic methylation reaction converts the neutral framework into a cationic one (ACOF-1R), in which the pyridinium- $N^+$  sites exhibit high binding free energy toward  $I_3^-$ , enabling selective and rapid adsorption. In addition, the high porosity of the material ensures efficient mass transfer of iodine species. Based on these features, the material achieves efficient capture and separation of both gaseous iodine species ( $I_2/CH_3I$ ) and liquid-phase iodine ( $I_3^-$ ). Precise control of the pore size in frameworks enhances iodine capture and improves performance. Hao *et al* [23] introduced a simple and general COF pore allocation strategy, successfully applying the porous pore-partitioned COFs to  $I_2$  and  $CH_3I$  capture (figure 1(c)). This strategy allows tailoring of the pore size of COFs to achieve pre-designed pore sizes, components and functions. In breakthrough tests, COF 3-2P dynamically adsorbed  $I_2$  and  $CH_3I$  more strongly than the non-partitioned parent COF (COF 3), reaching impressive loadings of 1.01 and 0.60  $\text{g g}^{-1}$  at 75 °C, respectively. Further, COF 3-2P exhibited high  $I_2$  and  $CH_3I$  uptake capacities of 0.42 and 0.24  $\text{g g}^{-1}$  at 150 °C, thus demonstrating excellent thermal stability. This work is the first to report the use of symmetrical building blocks to achieve spatial partitioning within COFs, thereby modifying the internal pore environment and introducing a higher density of nitrogen-rich sites, specifically triazine N-sites. Efficient iodine capture and speciation transformation ( $I_2 \rightarrow I_3^-/I_5^-$ ) are realized through charge-transfer interactions involving the triazine

N-sites. XPS and Raman spectroscopy confirm the electron transfer from nitrogen atoms to  $I_2$ , while DFT calculations further identify the triazine N-sites as the key active sites for the adsorption of both  $I_2$  and  $CH_3I$ . Wang *et al* [24] developed a novel ferrocene-functionalized POP (FeTz-POP) for efficient capture of radioactive iodine vapor from nuclear power plant emissions. The material exhibited an outstanding iodine uptake of 396 wt% at 75 °C under ambient pressure, which is 1.8 times higher than the ferrocene-free control (BpTz-POP). This enhancement is attributed to the stronger interaction between the cyclopentadienyl rings of ferrocene and iodine compared to benzene rings, the electrostatic binding of  $Fe^{2+}$  to polyiodide species ( $I_3^-/I_5^-$ ), and synergistic contributions from N-rich heterocycles and  $\pi$ -conjugated aromatic domains. This study not only introduces a high-performance iodine adsorbent but also offers a new strategy for functionalizing amorphous porous materials. The above studies demonstrate that the combination of strategies such as molecular design, surface functionalization, and fine-tuning of pore architectures are key research directions that can enhance both iodine capture efficiency and material stability.

POCs have unique structures and properties, which make them promising candidates for addressing iodine capture problems. Mao *et al* [25] proposed a feasible and efficient three-step post-synthetic modification (PSM) strategy to modify a representative POC (CC3). By integrating three iodine capture strategies via a PSM to enhance  $I_2$  affinity (figure 1(d)), the optimized POC (OFT-RCC3 $^{6+}6Br^-$ ) generates strong interactions between the  $Br^-$  anion and  $I_2/I_5^-$ . During the adsorption process,  $I_5^-$  tends to dissociate into  $I_3^-$  and  $I_2$ , forming a more stable  $I_2 \cdots Br^-$  interaction, which significantly promotes iodine uptake. Additionally, the positively charged cage framework enhances the electrostatic attraction toward  $I_3^-$ , resulting in an increase in binding energy by more than 130%. These two factors synergistically contribute to the efficient capture and transformation of multiple iodine species ( $I_2$ ,  $I_3^-$ , and  $I_5^-$ ). This synergistic design significantly enhanced iodine vapor uptake, establishing the modified POC as an ideal molecular container for  $I_2$  capture. Laboratory studies often differ from industrial environments, where complex systems, variable conditions, and stringent economic and technical requirements pose greater challenges to material performance. Liu *et al* [26] developed an effective platform for the efficient capture of radioactive iodine using POCs under industrial conditions (typically  $\geq 150$  °C,  $\leq 150$  ppmv  $I_2$ ) (figure 2(a)). Due to the highly dispersed and accessible binding sites within the POC, along with sufficient space to accommodate  $I_2$ , the constructed NKPOC-DT( $I^-$ ) exhibited a record-breaking  $I_2$  uptake capacity of 48.35 wt%. This performance surpasses the industrial silver-based adsorbent Ag@MOR and benchmark materials TGDM and 4F-iCOF-TpBpy- $I^-$  by factors of 3.5, 1.6, and 1.3, respectively, under identical conditions. The material outperforms neutral Lewis base-dominated systems, owing to the presence of ionic sites ( $N^+-CH_3I^-$ ). These ionic sites preferentially adsorb  $I_2$  via strong Coulombic interactions, with a binding energy of  $-1.14$  eV, which is 2.5 times higher than that of the Lewis base site (N). This enhanced interaction facilitates chemisorption of iodine and enables efficient capture even under high-temperature conditions. This work provides new insights into enhancing the adsorption capacity per unit ion-binding site, offering a promising strategy for improving iodine capture efficiency. Wang *et al* [27] synthesized porphyrin-based POCs (PTC-2 H and PTC-Zn) via dynamic covalent chemistry for the efficient capture of radioactive iodine from nuclear power plants. PTC-2 H exhibited an exceptionally high iodine uptake of  $5.46$  g g $^{-1}$ , attributed to the synergistic chemical adsorption provided by the large  $\pi$ -conjugated porphyrin plane, the  $-NH$  groups within the  $N_4$  cavity, and imine linkages. Upon zinc modification, the iodine uptake decreased to  $4.96$  g g $^{-1}$  due to the loss of  $-NH$  groups. This study is the first to highlight the critical role of porphyrin  $-NH$  sites





**Figure 2.** (a) The ‘highly dispersed’ and ‘readily accessible sites’ in POC can provide sufficient accommodation space for adsorbing more  $I_2$  molecules, thus effectively improving the adsorption ability of unit ionic sites. [26] John Wiley & Sons. © 2024 Wiley-VCH GmbH. (b) Construction of 2D  $(Cu(pyz)TiF_6)_n$  layers with type 2 pyz ligands to form quasi-3D networks in SCU-20 (pyz = pyrazine) and schematic illustration of the highly accessible active sites and slide rail-like 1D channels of SCU-20. Adapted from [29], with permission from Springer Nature. (c) A size-controllable nanosheet silicalite-1 zeolite, NSL-1, was designed for efficient and simultaneous capture of iodine and methyl iodide from nuclear waste. Adapted from [20], copyright (2024), with permission from Elsevier. (d) Flow chart of the synthetic steps for metal-modified BN aerogels. Adapted from [21], copyright (2023), with permission from Elsevier.

in enhancing iodine adsorption performance. In order to solve the problems of organic cage in actual use, it is difficult to fully utilize the active sites in solid state and not easy to recycle in liquid state. Cheng *et al* [28] synthesized four 2D COFs (Cage-TFB-COF, Cage-NTBA-COF, Cage-TFPB-COF, and Cage-TFPT-COF) by condensing a nitrogen-rich organic cage with four three-tooth linkers via Schiff-base polymerization. These COFs adopt AA stacking to form crystalline porous solids with 1D hexagonal channels, enhancing the accessibility of active sites in the solid state. Notably, Cage-NTBA-COF achieved an exceptional iodine uptake of 304 wt%, 14 times higher than the pristine cage solid. Spectroscopic analyses (FT-IR, XPS, and Raman) confirmed charge transfer interactions between iodine and the imine ( $C=N$ ) and aromatic ( $C=C/C-H$ ) moieties, leading to the formation of  $I_3^-$  and  $I_5^-$  polyiodides. This work demonstrates a tunable porous framework strategy for efficient iodine capture and speciation in both liquid and vapor phases.

Methyl iodide is typically immobilized through a methylation reaction, with most studies focusing on the use of post-modification strategies to introduce high-affinity functional groups inside porous adsorbents. However, this process carries the risk of blocking the material’s original pores, which may hinder the uptake of methyl iodide leading to poor overall adsorption performance. Therefore, an efficient  $CH_3I$  adsorbent should possess flexible channels, allowing optimal access of  $CH_3I$  to all active sites. Tai *et al* [29] developed a two-dimensional intercalated layered framework material (SCU-20). This material utilizes ‘rail-like’ pores and elastic interlayer contraction properties to trap methyl iodide within the framework via its accessible high-density active sites (figure 2(b)). The static adsorption capacity of SCU-20 for  $CH_3I$  is  $1.84\text{ g g}^{-1}$  ( $RH = 18\%$ ), and its adsorption performance is almost unaffected by high-dose radiation and environmental humidity. In SCU-20,  $CH_3I$  physisorption is primarily governed by exposed F sites, with strong electrostatic interactions of  $F-CH_3$  ( $-13.93\text{ kcal mol}^{-1}$ ) and  $F-I$  ( $-10.71\text{ kcal mol}^{-1}$ ), both significantly stronger than those at N sites ( $-5.83\text{ kcal mol}^{-1}$ ). Chemisorption occurs via

direct methylation of uncoordinated N atoms on the pyrazine rings. These two modes act synergistically, together with the material's unique interlayer groove structure, to enable high-capacity CH<sub>3</sub>I capture. To address the weak intermolecular interactions of CH<sub>3</sub>I, the active sites of adsorbent materials can be tailored to interact with the non-polar ( $\cdots\text{CH}_3$ ) and polar ( $\cdots\text{I}$ ) parts of CH<sub>3</sub>I, maximizing its capture. Jie *et al* [15] reported a multi-micro POP (MHP-P5Q), which is capable of fast adsorption of CH<sub>3</sub>I with a high adsorption capacity by utilizing CH $\cdots\pi$  interactions, halogen bonding ( $-\text{I}\cdots\text{N}=\text{C}-$ ) between imine groups and CH<sub>3</sub>I, and chemisorption within the microporous framework triple mechanism works together and combines a multi-level pore structure. Under high-temperature conditions, enhancing the interaction between the adsorbent and CH<sub>3</sub>I is also crucial for effective capture. Pan *et al* [30] developed an adsorbent, MFU-Cu(I), containing Cu(I) sites, which achieved a CH<sub>3</sub>I uptake in excess of 0.14 g g<sup>-1</sup> at 0.01 bar and 150 °C, exceeding the properties of various baseline adsorbents. Polar solvents could then efficiently remove CH<sub>3</sub>I adsorbed on Cu(I) sites, restoring the adsorption capacity of MFU-Cu(I), realize the regeneration of materials. MFU-Cu(I) efficiently captures CH<sub>3</sub>I through non-dissociative chemisorption at coordinatively unsaturated Cu(I) sites, generated via formate reduction, where the iodine end binds to Cu. EXAFS confirms the formation of Cu-I bonds upon adsorption. Its reversible adsorption behavior and stability at low CH<sub>3</sub>I concentrations highlight its potential as a functional material for radioactive methyl iodide remediation. Gao *et al* [31] developed a novel MOF, Ag-Tipe, for efficient capture of radioactive I<sub>2</sub> and CH<sub>3</sub>I from nuclear power plant emissions. At 75 °C, the material achieved high uptake capacities of 3.31 g g<sup>-1</sup> for I<sub>2</sub> and 0.55 g g<sup>-1</sup> for CH<sub>3</sub>I. The open Ag<sup>+</sup> sites enable direct coordination with iodine species to form AgI, while densely distributed imidazole groups enhance I<sub>2</sub> affinity via charge transfer and undergo methylation reactions with CH<sub>3</sub>I. Notably, Ag-Tipe exhibits excellent hydrophobicity, effectively resisting water vapor interference, making it highly promising for practical applications. These works demonstrate the importance of designing materials that can exploit specific CH<sub>3</sub>I-adsorbent interactions.

Organic porous materials are invaluable in iodine capture due to their flexible design, tunable pore sizes, and functionalization capabilities. Meanwhile, inorganic porous materials have attracted significant attention in this field due to their well-ordered pore structures, high specific surface areas, and diverse chemical compositions. Zhao *et al* [20] developed a hydrophobic nanosheet silicalite-1 (NSL-1) zeolite with tunable size for the efficient adsorption of I<sub>2</sub> and CH<sub>3</sub>I (figure 2(c)). By controlling particle size parameters to achieve an ultrathin structure and enhanced porosity, NSL-1 exhibits outstanding adsorption capacity and rapid kinetics, with an I<sub>2</sub> uptake of 553 mg g<sup>-1</sup> within 45 min and a CH<sub>3</sub>I uptake of 262 mg g<sup>-1</sup> within 1 h. Impressively, its hydrophobicity, acid resistance, and oxidation stability endow it with a higher iodine uptake capacity than conventional aluminosilicate zeolites. NSL-1 preferentially captures I<sub>2</sub> through a micropore confinement effect. XPS analysis indicates that I<sub>2</sub> and CH<sub>3</sub>I are adsorbed in molecular (I 3d<sub>5/2</sub> at 620.7 eV) and methyl iodide (I 3d<sub>5/2</sub> at 619.9 eV) forms, respectively, with iodine species uniformly distributed throughout the material. The physisorption-dominated mechanism retains its selectivity even under complex gas environments containing H<sub>2</sub>O and NO<sub>2</sub>, making NSL-1 a highly stable adsorbent for radioactive iodine removal. Additionally, the low cost and scalable synthesis of NSL-1 highlight its potential applications in the nuclear industry. However, the physical adsorption mechanism of inorganic porous materials may lead to a high iodine release rate, posing potential environmental concerns that require further investigation and optimization. Other research indicates that introducing metal active sites is another effective strategy for enhancing iodine capture performance. Unlike

purely physical adsorption mechanisms based on pore confinement effects, metal active sites can significantly improve the selectivity and adsorption capacity of materials for iodine through chemical bonding. Li *et al* [21] successfully synthesized a metal-modified boron nitride (BN) aerogel iodine adsorbent via a metal-induced, ultrasonic-assisted, and *in-situ* conversion method, thereby enhancing its iodine adsorption capacity (figure 2(d)). The high specific surface area and large pore volume of BN aerogels facilitate physical adsorption of I<sub>2</sub>, while the incorporation of Cu and Ag nanoparticles provides additional chemisorption sites. DFT calculations confirm that metal doping significantly enhances adsorption performance, attributed to the synergistic electron-donating effect of electron-rich nitrogen in h-BN and the free electrons from the metal sites in interacting with iodine species. Moreover, both ‘host–guest’ (adsorption site–I<sub>2</sub>) and ‘guest–guest’ (I<sub>2</sub>–I<sub>2</sub>) interactions coexist during the adsorption process, with metal sites primarily facilitating the initial adsorption stage by strengthening the host–guest interaction. As a result, BN–Cu and BN–Ag aerogels exhibit extraordinarily high iodine uptake capacities of 1739.8 wt.% and 2234.13 wt.%, respectively. Based on the unique advantages of BN materials, Li *et al* [32] developed a three-dimensional BN foam for the capture and reversible storage of iodine in both gaseous and liquid phases. This novel material, composed of porous BN microfibers, exhibits a high porosity and a large specific surface area of up to 561.92 m<sup>2</sup> g<sup>−1</sup>. The unique interwoven fibrous structure provides abundant  $\pi$ -conjugated domains and functional adsorption sites, enabling excellent iodine uptake with a maximum adsorption capacity of 212 wt% for gaseous iodine. In addition, the material retains the high thermal stability and chemical inertness characteristic of h-BN, allowing regeneration at 800 °C under a nitrogen atmosphere. Its monolithic foam structure offers practical advantages over conventional powdered adsorbents for applications in nuclear industry environments. These results highlight the great potential of BN foam for iodine adsorption and storage. However, in practical applications, this strategy may face challenges due to the uneven distribution of active sites on the material surface or the incomplete utilization of certain sites during interactions with iodine molecules. Consequently, further optimization is required to fully exploit their adsorption capacity for iodine.

To summarize, MOFs, COFs, POCs, and inorganic porous materials exhibit strong adsorption capabilities for iodine due to their tunable pore structures and high surface areas. Despite their remarkable iodine uptake capacities, many porous organic adsorbents have limited thermal stability which restricts their practical application in high-temperature environments. Furthermore, the presence of acidic water vapor in iodine-laden emissions from the nuclear industry poses additional challenges, as organic adsorbents generally lack chemical inertness and hydrophobicity, making them susceptible to degradation under such conditions. Additionally, most iodine adsorbents are synthesized in powder form, which complicates their collection and increases the risk of secondary environmental contamination due to particle dispersion. Therefore, developing highly efficient and stable solid-state iodine adsorbents with enhanced durability and processability remains a critical challenge for practical applications.

### 3. Perspective

Although substantial progress has been made in the design, development and performance optimization of porous materials for iodine capture, challenges such as the long-term stability of the materials and scalability for practical applications remain. Solid materials, cutting-edge technologies, intelligent computing, and interdisciplinary collaboration can drive advancements in iodine capture.



Specifically: (i) material design—hybrid materials combining polymers and nanoparticles offer high adsorption capacity, chemical versatility, and durability, making them suitable for both gaseous and aqueous iodine containment. For gaseous iodine control, flexible polymer–nanoparticle composites can be integrated into filtration systems. In aqueous systems, a careful balance of hydrophilicity and hydrophobicity is crucial. Future research should focus on surface chemistry modifications of nanoparticles to selectively bind iodine even in the presence of competing ions and organic matter. Also, layered double hydroxides with anion-exchange capabilities can be modified to capture iodine species from radioactive waste streams. Their structural versatility allows the incorporation of iodine into their interlayer spaces, forming stable complexes that minimize iodine mobility; (ii) at the technical level, electrochemical and photocatalytic technologies offer new approaches for iodine capture. Electrochemical techniques using redox-active electrodes can selectively capture and separate iodine species in complex aqueous or gaseous environments. By tuning the electrode potential, these systems can efficiently extract iodine without the need for chemical reagents, reducing secondary waste generation. Advanced photocatalysts, such as heterostructured semiconductors, can utilize sunlight or artificial light to oxidize iodide ( $I^-$ ) into less mobile iodate ( $IO_3^-$ ) or reduce volatile molecular iodine ( $I_2$ ) into stable iodide species. This process stabilizes iodine and provides a sustainable, energy-efficient approach to iodine management; (iii) leveraging machine learning and high-throughput computational simulations, researchers can design next-generation materials with optimized properties for iodine capture and containment. Computational tools enable the prediction of adsorption capacities, material stability, and interaction mechanisms, accelerating the development cycle for novel solutions; (iv) the integration of multiple disciplines, including physics, chemistry, and biology, should enable the development of more precise and efficient iodine capture systems. For instance, combining microfluidic technology with advanced adsorbents can achieve high-efficiency iodine enrichment and rapid separation. In summary, the integration of advanced materials, cutting-edge technologies, and algorithm-driven approaches, coupled with interdisciplinary collaboration, holds the potential to establish comprehensive solutions encompassing detection, separation, and immobilization. This will provide a robust foundation for the long-term safe management of radioactive iodine while driving radionuclide remediation technologies toward greater efficiency, sustainability, and intelligence.

### Data availability statement

No new data were created or analyzed in this study.

### Acknowledgments

We acknowledge funding from the National Natural Science Foundation of China (Grants 22322603, U2167218, 22341602, U2341289), the Beijing Outstanding Young Scientist Program. G.I.N.W. acknowledges funding support from the MacDiarmid Institute for Advanced Materials and Nanotechnology. S. M. acknowledges the Robert A. Welch Foundation (B-0027).

### Conflict of interest

The authors declare no conflict of interest.

## ORCID iDs

Geoffrey I N Waterhouse  <https://orcid.org/0000-0002-3296-3093>

Xiangke Wang  <https://orcid.org/0000-0002-3352-1617>

## References

- [1] Riley B J, Vienna J D, Strachan D M, McCloy J S and Jerden J L 2016 Materials and processes for the effective capture and immobilization of radioiodine: a review *J. Hazard. Mater.* **470** 307–26
- [2] He L *et al* 2021 A nitrogen-rich covalent organic framework for simultaneous dynamic capture of iodine and methyl iodide *Chem* **7** 699–714
- [3] Zhang M, Samanta J, Atterberry B A, Staples R, Rossini A J and Ke C 2022 A crosslinked ionic organic framework for efficient iodine and iodide remediation in water *Angew. Chem., Int. Ed.* **61** e202214189
- [4] Huve J, Ryzhikov A, Nouali H, Lalia V, Auge G and Daou T J 2018 Porous sorbents for the capture of radioactive iodine compounds: a review *RSC Adv.* **8** 29248–73
- [5] Zheng B, Liu X, Hu J, Wang F, Hu X, Zhu Y, Lv X, Du J and Xiao D 2019 Construction of hydrophobic interface on natural biomaterials for higher efficient and reversible radioactive iodine adsorption in water *J. Hazard. Mater.* **368** 81–89
- [6] Tian Z, Chee T S, Zhu L, Duan T, Zhang X, Lei L and Xiao C 2021 Comprehensive comparison of bismuth and silver functionalized nickel foam composites in capturing radioactive gaseous iodine *J. Hazard. Mater.* **417** 125978
- [7] Zhou Y-R, Wang S-L, Zhang L, Fu J, He L and Tao G-H 2024 Electronic-rich large conjugated molecules dispersing through ionic liquid solution process for fluorescent detection of iodine gas *Chem. Eng. J.* **492** 152075
- [8] Xie L, Zheng Z, Lin Q, Zhou H, Ji X, Sessler J L and Wang H 2022 Calix[4]pyrrole-based crosslinked polymer networks for highly effective iodine adsorption from water *Angew. Chem., Int. Ed.* **61** e202113724
- [9] Xie Y *et al* 2024 Engineering the pore environment of antiparallel stacked covalent organic frameworks for capture of iodine pollutants *Nat. Commun.* **15** 2671
- [10] Kang H W, Choi J-H, Lee K R and Park H-S 2021 Addition of transition metal oxides on silver tellurite glass for radioactive iodine immobilization *J. Nucl. Mater.* **543** 152635
- [11] Chong S, Peterson J A, Riley B J, Tabada D, Wall D, Corkhill C L and McCloy J S 2018 Glass-bonded idosodalite waste form for immobilization of  $^{129}\text{I}$  *J. Nucl. Mater.* **504** 109–21
- [12] Soudani S, Gars L L, Morizet Y, Deniard P, Gautron E and Grolleau S 2023 High-pressure glass-ceramics for iodine nuclear waste immobilization: preliminary experimental results *Ceram. Int.* **49** 30029–38
- [13] Wang C *et al* 2017 A 3D covalent organic framework with exceptionally high iodine capture capability *Chem. Eur. J.* **24** 585–9
- [14] Wang Q, Tao Y, Li Z, Ye W, Wang Y, Liu D and He Y 2024 Visualizing dynamic competitive adsorption processes between iodine and methyl iodide within single covalent organic framework crystals *J. Hazard. Mater.* **463** 132841
- [15] Jie K *et al* 2020 Mechanochemical synthesis of pillar[5]quinone derived multi-microporous organic polymers for radioactive organic iodide capture and storage *Nat. Commun.* **11** 1086
- [16] Cao X, Jin Y, Wang H, Ding X, Liu X, Yu B, Zhan X and Jiang J 2024 A tetraaldehyde-derived porous organic cage and covalent organic frameworks: syntheses, structures, and iodine vapor capture *Chin. Chem. Lett.* **35** 109201
- [17] O'Shaughnessy M, Glover J, Hafizi R, Barhi M, Clowes R, Chong S Y, Argent S P, Day G M and Cooper A I 2024 Porous isorecticular non-metal organic frameworks *Nature* **630** 102–8
- [18] Li B *et al* 2017 Capture of organic iodides from nuclear waste by metal-organic framework-based molecular traps *Nat. Commun.* **8** 485
- [19] Pham T C T, Docao S, Hwang I C, Song M K, Choi D Y, Moon D, Oleynikov P and Yoon K B 2016 Capture of iodine and organic iodides using silica zeolites and the semiconductor behaviour of iodine in a silica zeolite *Energy Environ. Sci.* **9** 1050–62
- [20] Zhao Q, Li X, Chen G, Wang Z, Tan C, Liu C, Zou H, Ma J, Zhu L and Duan T 2024 Hydrophobic nanosheet silicalite-1 zeolite for iodine and methyl iodide capture *J. Hazard. Mater.* **472** 134496
- [21] Li G, Liang J, Lin J, Li H, Liu Y, Xu G, Yu C, Guo Z, Tang C and Huang Y 2023 Boron nitride aerogels incorporated with metal nanoparticles: multifunctional platforms for iodine capture and detection *J. Hazard. Mater.* **460** 132481
- [22] Guo X, Li Y, Zhang M, Cao K, Tian Y, Qi Y, Li S, Li K, Yu X and Ma L 2020 Colyliform crystalline 2D covalent organic frameworks (COFs) with Quasi-3D topologies for rapid  $\text{I}_2$  adsorption *Angew. Chem., Int. Ed.* **59** 22697–705

- [23] Hao M, Xie Y, Lei M, Liu X, Chen Z, Yang H, Waterhouse G I N, Ma S and Wang X 2023 Pore space partition synthetic strategy in imine-linked multivariate covalent organic frameworks *J. Am. Chem. Soc.* **146** 1904–13
- [24] Wang Y, Tao J, Xiong S, Lu P, Tang J, He J, Javaid M U, Pan C and Yu G 2020 Ferrocene-based porous organic polymers for high-affinity iodine capture *Chem. Eng. J.* **380** 122420
- [25] Mao Q, Yang S, Zhang J, Liu Y and Liu M 2024 Post-synthetic modification of porous organic cages for enhanced iodine adsorption performance *Adv. Sci.* **11** e2408494
- [26] Liu X *et al* 2024 Porous organic cage as an efficient platform for industrial radioactive iodine capture *Angew. Chem., Int. Ed.* **63** e202411342
- [27] Wang Z, Li J, Du Z, Pang L and Liu C 2025 Metal-free porphyrin porous organic cage for efficient iodine capture *Chem. Eng. J.* **509** 161326
- [28] Cheng K, Li H, Wang J R, Li P Z and Zhao Y 2023 From supramolecular organic cages to porous covalent organic frameworks for enhancing iodine adsorption capability by fully exposed nitrogen-rich sites *Small* **19** e2301998
- [29] Tai B *et al* 2024 Flexible interdigitated layered framework with multiple accessible active sites for high-performance CH<sub>3</sub>I capture *Sci. China Chem.* **67** 1569–77
- [30] Pan T, Yang K, Dong X, Zuo S, Chen C, Li G, Emwas A H, Zhang H and Han Y 2024 Strategies for high-temperature methyl iodide capture in azolate-based metal-organic frameworks *Nat. Commun.* **15** 2630
- [31] Gao X, Hu Q H, Shi Y Z, Liang R P and Qiu J D 2025 Synthesis of an Ag-based metal-organic framework for effective capture of iodine pollutants *Sep. Purif. Technol.* **359** 130353
- [32] Li G, Huang Y, Lin J, Yu C, Liu Z, Fang Y, Xue Y and Tang C 2020 Effective capture and reversible storage of iodine using foam-like adsorbents consisting of porous boron nitride microfibers *Chem. Eng. J.* **382** 122833