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Research Article

Defect Engineering in Transition Metal Oxides for Energy, Environmental, and Materials Technology Applications: A Comprehensive Review

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ABSTRACT

Transition metal oxides (TMOs) have emerged as one of the most promising classes of functional materials due to their outstanding electrical, optical, catalytic, and chemical properties. Their versatile characteristics make them highly suitable for applications in energy storage, photocatalysis, gas sensing, environmental remediation, and electronic devices. In recent years, defect engineering has become an effective strategy for enhancing the performance of transition metal oxides by tailoring their structural and electronic properties. Defects such as oxygen vacancies, interstitial atoms, surface defects, and dopant-induced imperfections significantly influence charge transport, light absorption, catalytic activity, and ion diffusion behavior. This review provides a comprehensive overview of defect engineering approaches in transition metal oxides and their impact on energy and environmental applications. The review discusses the fundamental concepts of crystal defects, synthesis techniques, and advanced characterization methods used to investigate defect structures in metal oxides. Various defect engineering strategies, including oxygen vacancy generation, elemental doping, surface modification, heterostructure formation, and strain engineering, are critically analyzed. Furthermore, the review highlights recent developments in photocatalysis, lithium-ion batteries, supercapacitors, gas sensors, and optoelectronic devices based on defect-engineered metal oxides. The major challenges related to structural stability, scalability, and environmental sustainability are also discussed. Finally, future research perspectives involving artificial intelligence-assisted materials design, multifunctional nanostructures, and green synthesis approaches are presented. This review aims to provide valuable insights into the role of defect engineering in advancing the performance and practical applications of transition metal oxide materials in modern technology.

Keywords: Transition metal oxides; defect engineering; oxygen vacancies; photocatalysis; energy storage

INTRODUCTION

BACKGROUND OF METAL OXIDES

Metal oxides represent one of the most important classes of inorganic materials widely investigated in materials science, chemistry, physics, and engineering due to their remarkable physical and chemical properties. These materials are formed through the combination of metal elements with oxygen atoms, resulting in stable compounds with diverse crystal structures and functionalities. Metal oxides exhibit excellent optical, electrical, magnetic, catalytic, and thermal characteristics, making them highly suitable for numerous industrial and technological applications. In recent years, metal oxides have gained increasing attention in advanced applications such as photocatalysis, gas sensing, energy conversion, environmental remediation, solar cells, batteries, and biomedical devices. Their low cost, chemical stability, environmental

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compatibility, and tunable electronic properties make them promising candidates for next-generation functional materials. The continuous advancement in nanotechnology and materials engineering has further accelerated research on metal oxides, particularly in the development of nanostructured and defect-engineered systems for enhanced performance.

TRANSITION METAL OXIDES

Transition metal oxides (TMOs) constitute a special category of metal oxides that contain transition metal elements such as titanium, zinc, iron, copper, nickel, cobalt, and cerium. These materials possess partially filled d-orbitals, which contribute significantly to their unique electronic, magnetic, catalytic, and optical properties. Unlike conventional oxides, TMOs can exhibit multiple oxidation states, enabling complex electron transfer processes and superior catalytic activities. Common transition metal oxides including titanium dioxide (TiO_2), zinc oxide (ZnO), iron oxide (Fe_2O_3), cerium oxide (CeO_2), and nickel oxide (NiO) have been extensively studied for applications in photocatalysis, supercapacitors, lithium-ion batteries, sensors, and fuel cells. Their electronic structures can be modified through doping, surface engineering, and defect manipulation, allowing researchers to tailor material properties according to specific applications. Due to these advantages, transition metal oxides have emerged as one of the most actively explored material systems in modern materials research.

WHY DEFECT ENGINEERING?

Defect engineering has become an essential strategy for improving the performance of transition metal oxides in various technological applications. In crystalline materials, defects refer to irregularities or imperfections in the atomic arrangement, including vacancies, interstitial atoms, dislocations, and grain boundaries. Among these, oxygen vacancies are considered one of the most influential defects in metal oxides because they strongly affect the electronic structure, conductivity, surface reactivity, and optical behavior of the materials. By intentionally introducing and controlling defects, researchers can significantly enhance charge transport, catalytic activity, ion diffusion, and light absorption properties. Defect engineering also enables better separation of electron-hole pairs in photocatalytic systems, thereby improving the efficiency of energy conversion and pollutant degradation processes. Furthermore, controlled defect formation can create active surface sites that facilitate gas adsorption and electrochemical reactions. As a result, defect engineering has become a powerful approach for optimizing the functional performance of transition metal oxides in energy storage, sensing, catalysis, and environmental applications.

SCOPE AND OBJECTIVES OF THE REVIEW

The primary objective of this review is to provide a comprehensive overview of defect engineering strategies in transition metal oxides and their influence on energy and environmental applications. This review discusses the fundamental concepts of defects, synthesis approaches, characterization techniques, and the mechanisms through which defects enhance material performance. Particular attention is given to oxygen vacancies, elemental doping, heterostructure formation, and surface modification methods used to tailor the electronic and catalytic properties of metal oxides. In addition, the review critically evaluates recent advances in photocatalysis, batteries, supercapacitors, gas sensors, and electronic devices based on defect-engineered materials. The current challenges associated with material stability, large-scale production, and environmental safety are also discussed. By summarizing recent developments and identifying future research directions, this review aims to provide valuable insights for researchers working in advanced materials science and nanotechnology.

FUNDAMENTALS OF METAL OXIDE DEFECTS

CRYSTAL STRUCTURES OF METAL OXIDES

The crystal structure of metal oxides plays a fundamental role in determining their physical, electronic, and chemical properties. Different atomic arrangements influence charge transport, defect formation, catalytic activity, and structural stability. Common crystal structures observed in transition metal oxides include rock

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salt, spinel, perovskite, and wurtzite structures. For example, zinc oxide commonly crystallizes in the hexagonal wurtzite structure, while titanium dioxide exists mainly in anatase and rutile phases. Perovskite oxides are widely studied for their excellent ionic conductivity and catalytic behavior in energy-related applications. The arrangement of metal and oxygen atoms within these crystal lattices directly affects the formation and mobility of defects such as oxygen vacancies and interstitial ions. Furthermore, crystal orientation, grain boundaries, and lattice distortion significantly influence the electronic band structure and surface chemistry of metal oxides. Therefore, understanding crystal structures is essential for designing defect-engineered materials with optimized performance. **Fig. 1** presents the common crystal structures of transition metal oxides, including rock salt, spinel, perovskite, and wurtzite structures, along with their coordination environments, representative materials, and key structural features influencing their physical and chemical properties.

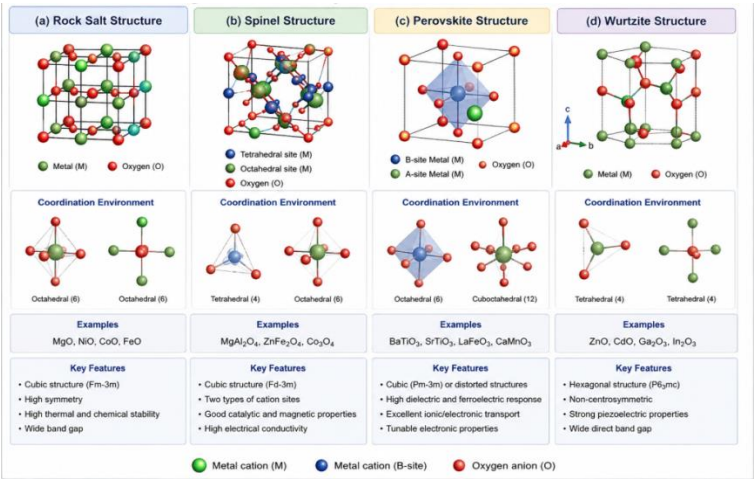


Figure 1. Schematic illustration of common crystal structures of transition metal oxides, including rock salt, spinel, perovskite, and wurtzite structures, showing their coordination environments, representative compounds, and key structural characteristics.

TYPES OF DEFECTS

Defects in metal oxides can be classified into several categories depending on their dimensionality and formation mechanism. Point defects are localized imperfections involving missing atoms, substituted atoms, or interstitial species within the crystal lattice. Oxygen vacancies, which occur when oxygen atoms are absent from their lattice positions, are among the most important point defects in transition metal oxides. Line defects, also known as dislocations, involve distortions along one-dimensional lattice lines and can affect mechanical and electrical properties. Surface defects arise from incomplete atomic coordination at the material surface and often serve as active sites for catalytic reactions and adsorption processes. Additionally, grain boundaries and planar defects contribute to changes in charge transport and ion diffusion. These defects can either occur naturally during synthesis or be intentionally introduced through thermal treatment, doping, irradiation, or chemical reduction. The presence and concentration of defects strongly influence the optical absorption, conductivity, reactivity, and electrochemical behavior of metal oxide materials. **Fig. 2** presents the major types of defects in transition metal oxides, including point defects, line defects, surface defects, and oxygen vacancies, illustrating their formation mechanisms and influence on the structural and electronic properties of metal oxide materials.

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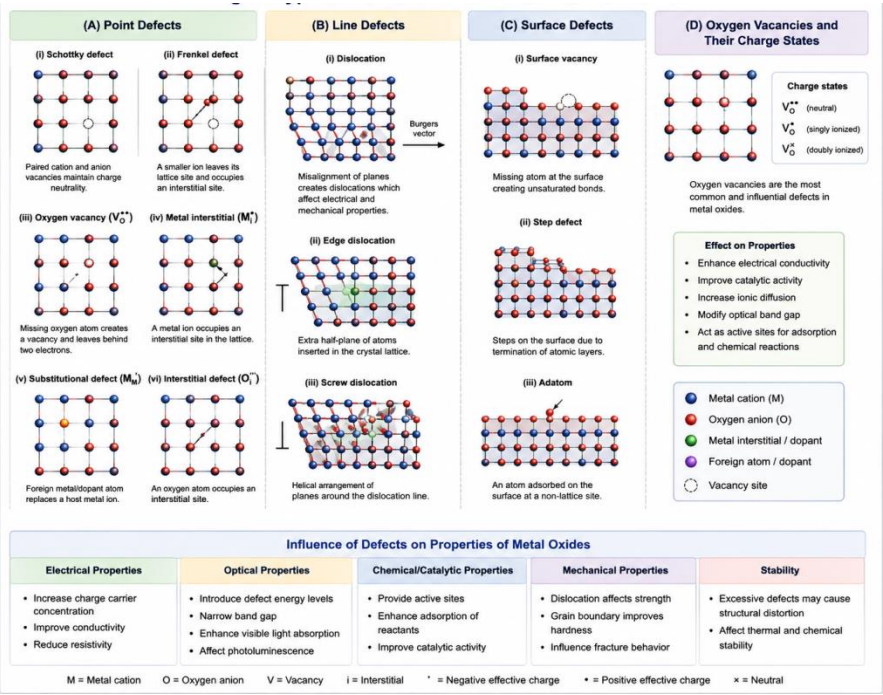


Figure 2. Schematic representation of different defect types in transition metal oxides, including vacancies, interstitial defects, substitutional defects, dislocations, grain boundaries, and surface defects affecting the physical, optical, and catalytic properties of metal oxide materials.

ELECTRONIC AND OPTICAL EFFECTS OF DEFECTS

Defects significantly alter the electronic and optical properties of transition metal oxides by modifying their electronic band structures and charge carrier dynamics. Oxygen vacancies and other point defects introduce localized energy levels within the band gap, enabling enhanced visible-light absorption and improved electrical conductivity. These defect states can act as electron donors, increasing free carrier concentration and facilitating charge transport within the material. In photocatalytic systems, defects help reduce the recombination rate of photogenerated electron-hole pairs, thereby improving photocatalytic efficiency. Furthermore, defect-induced band gap narrowing allows metal oxides to utilize a broader portion of the solar spectrum, which is highly beneficial for solar energy conversion and environmental remediation applications. Defects also influence optical phenomena such as photoluminescence, light scattering, and absorption intensity. However, excessive defect concentrations may lead to structural instability and undesired charge recombination, highlighting the importance of carefully controlling defect density to achieve optimal performance. **Fig. 3** presents a schematic representation of the influence of defect states on the electronic and optical properties of transition metal oxides. The introduction of intrinsic defects, such as oxygen vacancies, and extrinsic defects generated through doping creates localized energy levels within the forbidden bandgap. These defect states facilitate charge carrier trapping and transfer processes, enhance visible-light absorption through bandgap narrowing, and suppress electron-hole recombination. Consequently, defect-engineered metal oxides exhibit improved electrical conductivity, enhanced photocatalytic activity, increased carrier mobility, and superior optoelectronic performance compared with defect-free materials.

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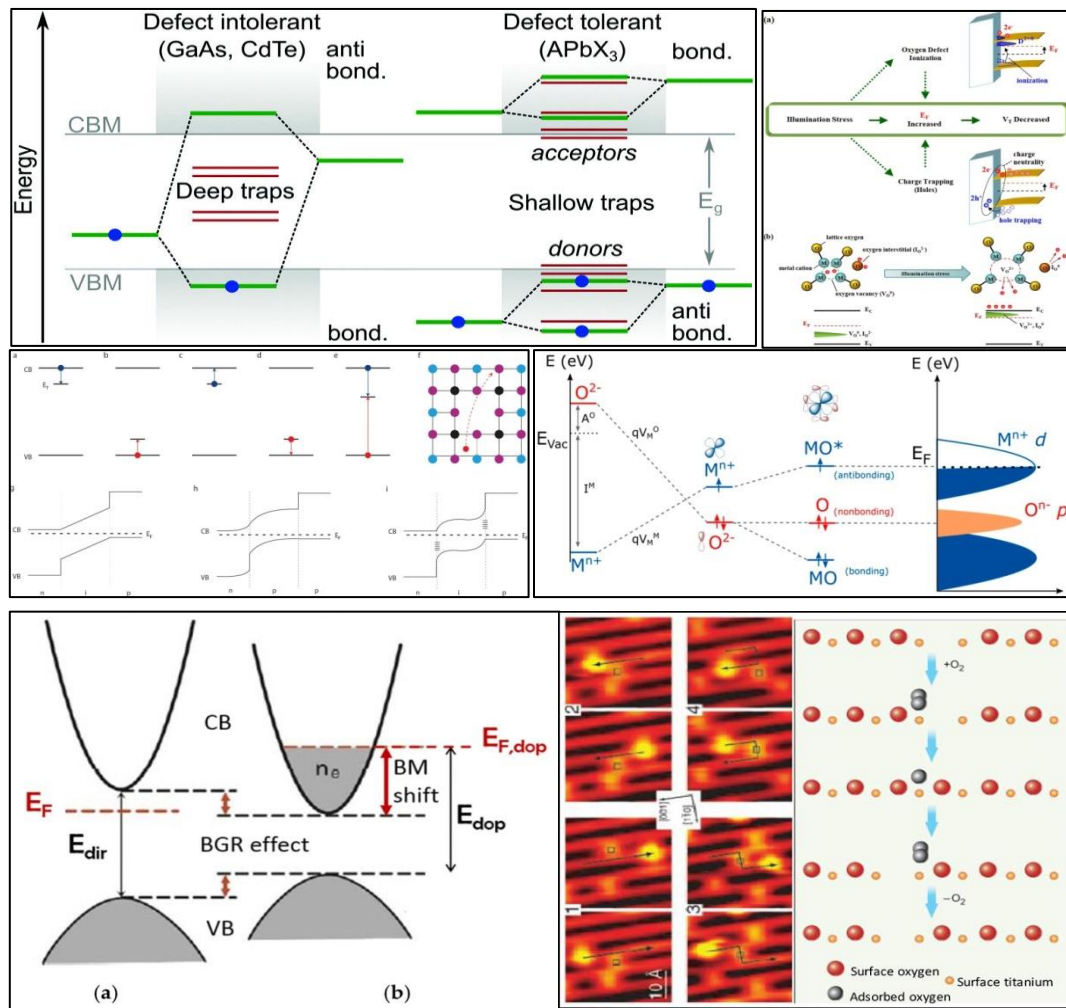


Fig. 3. Schematic illustration of the electronic and optical effects of defects in transition metal oxides: **(a)** electronic band structure of a pristine metal oxide showing the valence band (VB), conduction band (CB), and intrinsic bandgap; **(b)** formation of oxygen-vacancy-induced defect states within the bandgap; **(c)** bandgap narrowing and enhanced visible-light absorption resulting from defect engineering; **(d)** charge carrier generation and separation under light irradiation in defect-rich metal oxides; **(e)** suppression of electron-hole recombination through defect-mediated charge trapping; **(f)** enhanced charge transport and electrical conductivity due to increased carrier concentration; and **(g)** improved photocatalytic and optoelectronic performance arising from defect-induced electronic structure modifications.

CHARACTERIZATION TECHNIQUES

Advanced characterization techniques are essential for investigating the structural, morphological, chemical, and electronic properties of defect-engineered metal oxides. X-ray diffraction (XRD) is widely used to analyze crystal structure, phase composition, and lattice distortion resulting from defect formation. Scanning electron microscopy (SEM) and transmission electron microscopy (TEM) provide detailed information regarding surface morphology, particle size, and nanostructure features. X-ray photoelectron spectroscopy (XPS) is particularly important for identifying oxidation states and detecting oxygen vacancies or dopant elements on material surfaces. Raman spectroscopy is commonly employed to study lattice vibrations and structural disorder associated with defects. Additionally, photoluminescence (PL) spectroscopy and electron paramagnetic resonance (EPR) are highly effective techniques for analyzing electronic defect states and charge carrier behavior. Combining multiple characterization methods enables researchers to obtain a comprehensive understanding of defect formation mechanisms and their impact on material performance.

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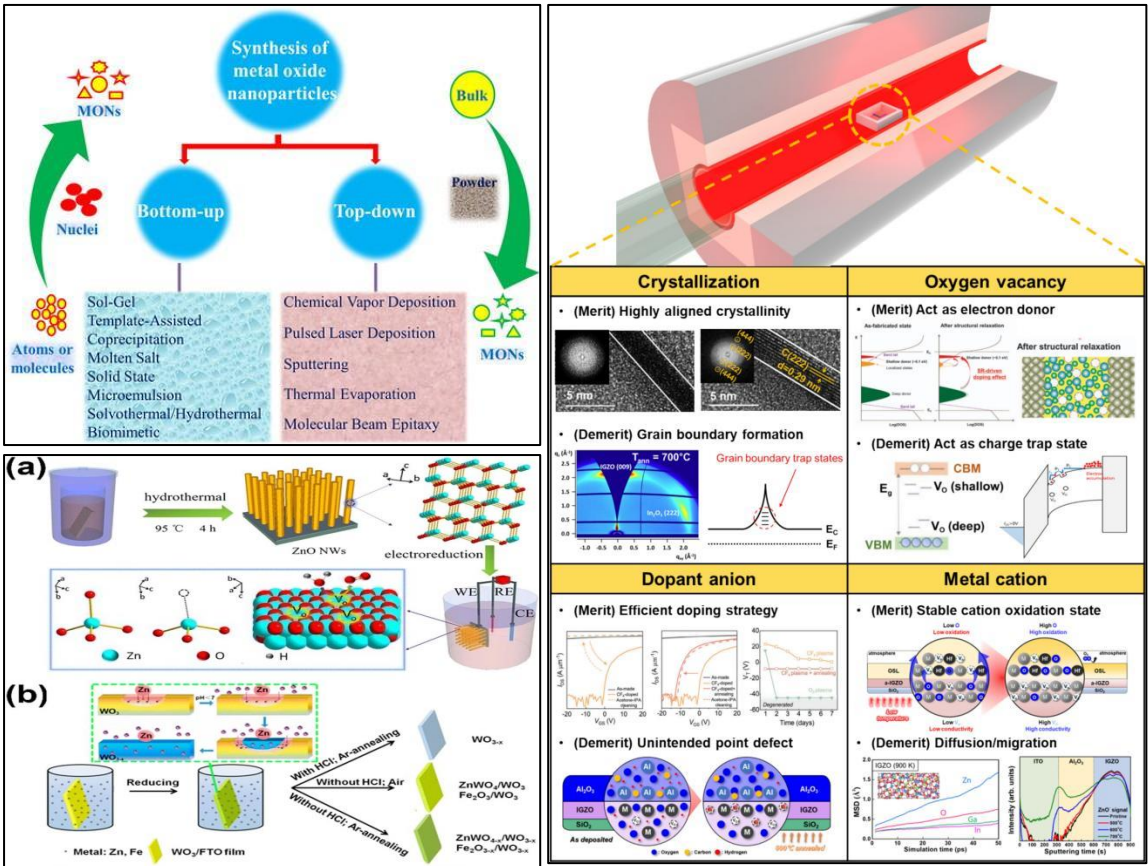
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SYNTHESIS METHODS FOR DEFECT-ENGINEERED METAL OXIDES

The synthesis method plays a crucial role in determining the structural, morphological, and electronic properties of defect-engineered metal oxides. Different preparation techniques influence particle size, crystallinity, surface area, defect concentration, and chemical composition, which ultimately affect the performance of metal oxides in various applications. In recent years, researchers have developed several synthesis approaches to precisely control defect formation and tailor material properties according to specific technological requirements. Methods such as sol-gel processing, hydrothermal synthesis, chemical vapor deposition, electrochemical synthesis, and green synthesis have gained significant attention due to their ability to produce highly efficient defect-engineered nanomaterials. Each technique offers unique advantages in terms of defect control, scalability, cost-effectiveness, and material uniformity. Therefore, understanding these synthesis methods is essential for optimizing the design and performance of transition metal oxide materials. **Fig. 4** presents the major synthesis approaches employed for the fabrication of defect-engineered transition metal oxides. The figure illustrates various physical, chemical, and post-treatment methods used to introduce and control defects such as oxygen vacancies, interstitial atoms, substitutional dopants, lattice distortions, and surface defects. Chemical synthesis techniques including sol-gel, hydrothermal, solvothermal, co-precipitation, and combustion methods enable defect formation during crystal growth, while post-synthesis treatments such as thermal annealing, hydrogen reduction, plasma treatment, laser irradiation, and ion implantation allow precise defect tuning after material formation. The controlled introduction of defects through these methods modifies the electronic structure, conductivity, optical absorption, catalytic activity, and surface reactivity of metal oxides, thereby enhancing their performance in energy, environmental, sensing, and biomedical applications.



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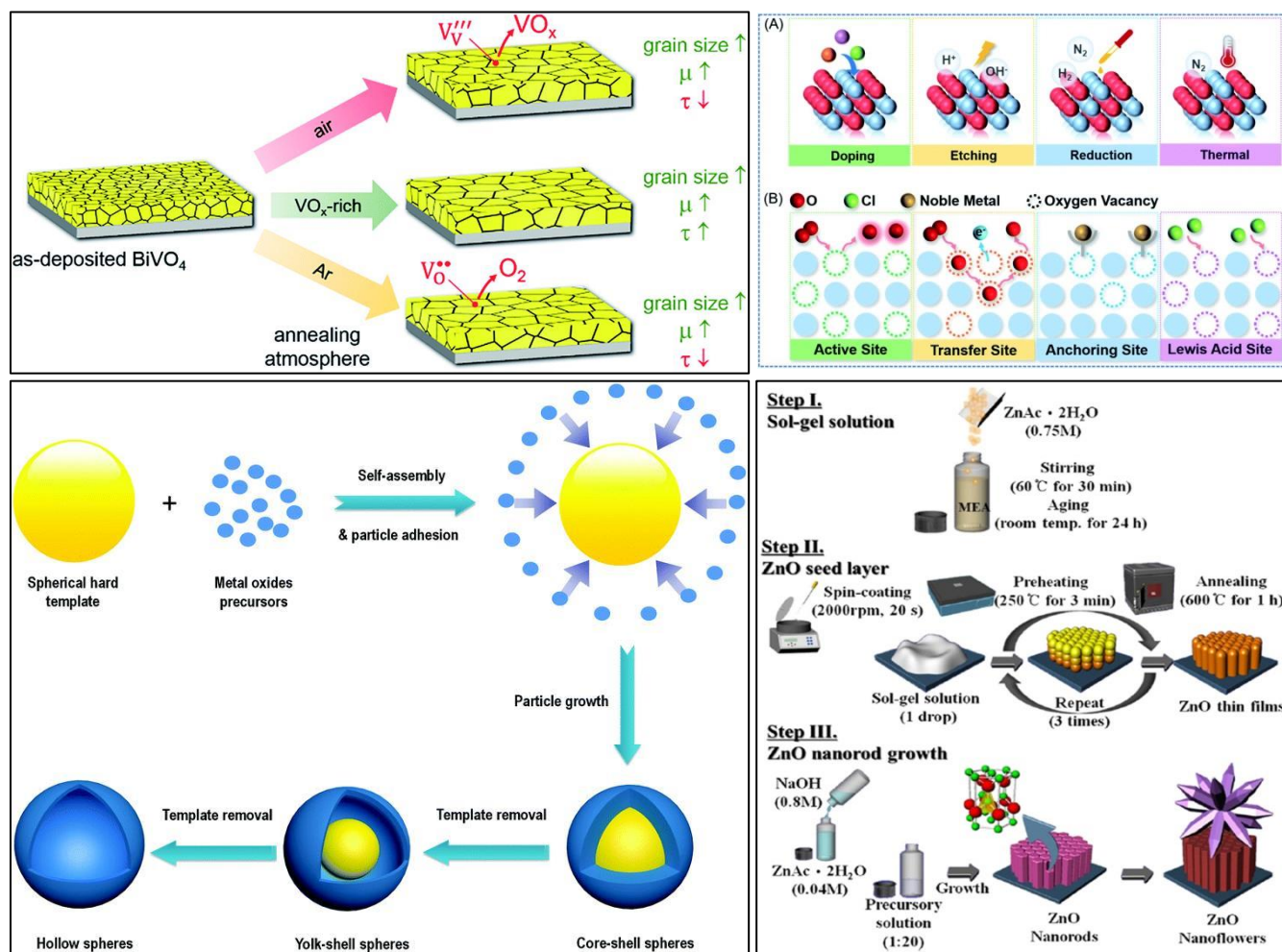


Fig. 4. Schematic representation of synthesis methods used for defect engineering in transition metal oxides: (a) sol-gel synthesis for controlled dopant incorporation and defect generation; (b) hydrothermal/solvothermal synthesis enabling defect-rich nanostructure formation; (c) co-precipitation and combustion methods for large-scale production of defect-engineered oxides; (d) thermal annealing under reducing or inert atmospheres for oxygen vacancy creation; (e) hydrogen reduction treatment for generating oxygen-deficient structures; (f) plasma and laser-assisted processing for surface defect engineering; (g) ion implantation and elemental doping for precise defect control; and (h) resulting defect-engineered metal oxides exhibiting tailored electronic, optical, catalytic, and electrochemical properties.

SOL-GEL METHOD

The sol-gel method is one of the most widely used chemical synthesis techniques for preparing defect-engineered metal oxides due to its simplicity, low processing temperature, and excellent compositional control. In this method, metal precursors such as metal alkoxides or metal salts undergo hydrolysis and condensation reactions to form a colloidal solution known as a sol, which gradually transforms into a gel network. The resulting gel is then dried and calcined to produce metal oxide nanoparticles or thin films. One of the major advantages of the sol-gel process is its ability to produce homogeneous materials with controlled particle size and high surface area. Additionally, defect concentration can be adjusted by modifying synthesis parameters such as pH, precursor concentration, calcination temperature, and reaction atmosphere. The sol-gel method is particularly suitable for introducing oxygen vacancies and dopants into transition metal oxides, thereby enhancing their catalytic, optical, and electrochemical properties. Due to its versatility and cost-effectiveness, the sol-gel method is extensively used in photocatalysis, sensors, coatings, and energy storage applications. **Fig. 5** presents the schematic workflow of the sol-gel synthesis method used for the fabrication of defect-engineered transition metal oxides. The process involves precursor

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solution preparation, hydrolysis, condensation, gel formation, drying, and calcination, resulting in crystalline metal oxide nanostructures. During these stages, defects such as oxygen vacancies, dopant-induced lattice distortions, and surface defects can be introduced and controlled to tailor the electronic, optical, catalytic, and electrochemical properties of the material.

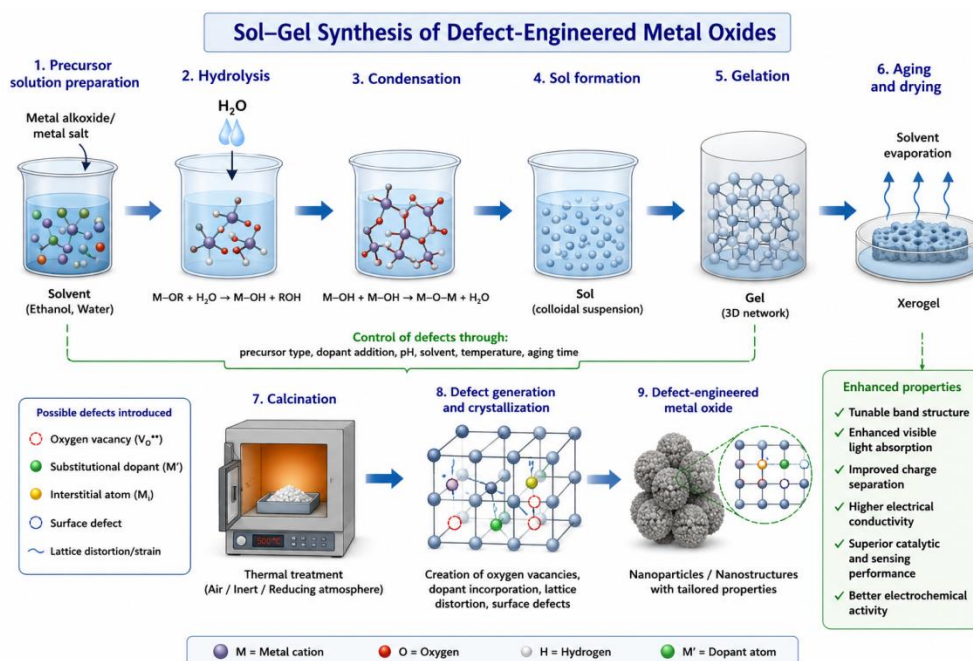


Fig. 5. Schematic illustration of the sol-gel synthesis route for defect-engineered transition metal oxides.

HYDROTHERMAL/SOLVOTHERMAL METHODS

Hydrothermal and solvothermal synthesis methods are highly effective techniques for producing defect-engineered metal oxides with controlled morphology and crystallinity. These methods involve chemical reactions in sealed autoclaves under high temperature and pressure conditions, where water or organic solvents act as the reaction medium. Hydrothermal synthesis uses water as the solvent, while solvothermal synthesis utilizes non-aqueous organic solvents. The elevated pressure and temperature facilitate crystal growth, phase formation, and defect generation within the metal oxide structure. These methods are particularly advantageous for synthesizing nanostructures such as nanorods, nanotubes, nanosheets, and hierarchical architectures with enhanced surface activity. By adjusting reaction parameters such as temperature, reaction time, solvent type, and precursor concentration, researchers can precisely control defect density and crystal morphology. Hydrothermal and solvothermal methods are widely employed in the synthesis of TiO_2 , ZnO , Fe_2O_3 , and CeO_2 nanomaterials for applications in photocatalysis, batteries, supercapacitors, and gas sensors. The ability to produce highly crystalline materials with tunable defects makes these methods highly valuable in advanced materials engineering. **Fig. 6** presents the hydrothermal/solvothermal synthesis process used for the fabrication of defect-engineered transition metal oxides. In this method, metal precursors are dissolved in water (hydrothermal) or organic solvents (solvothermal) to form a homogeneous solution. The solution is then transferred into a sealed autoclave and subjected to elevated temperature and pressure, promoting nucleation and crystal growth. The reaction conditions, including temperature, pressure, solvent type, reaction time, and precursor concentration, strongly influence defect formation. Oxygen vacancies, dopant incorporation, lattice distortions, and surface defects can be effectively introduced during crystal growth, resulting in metal oxide nanostructures with enhanced structural, electronic, optical, catalytic, and electrochemical properties.

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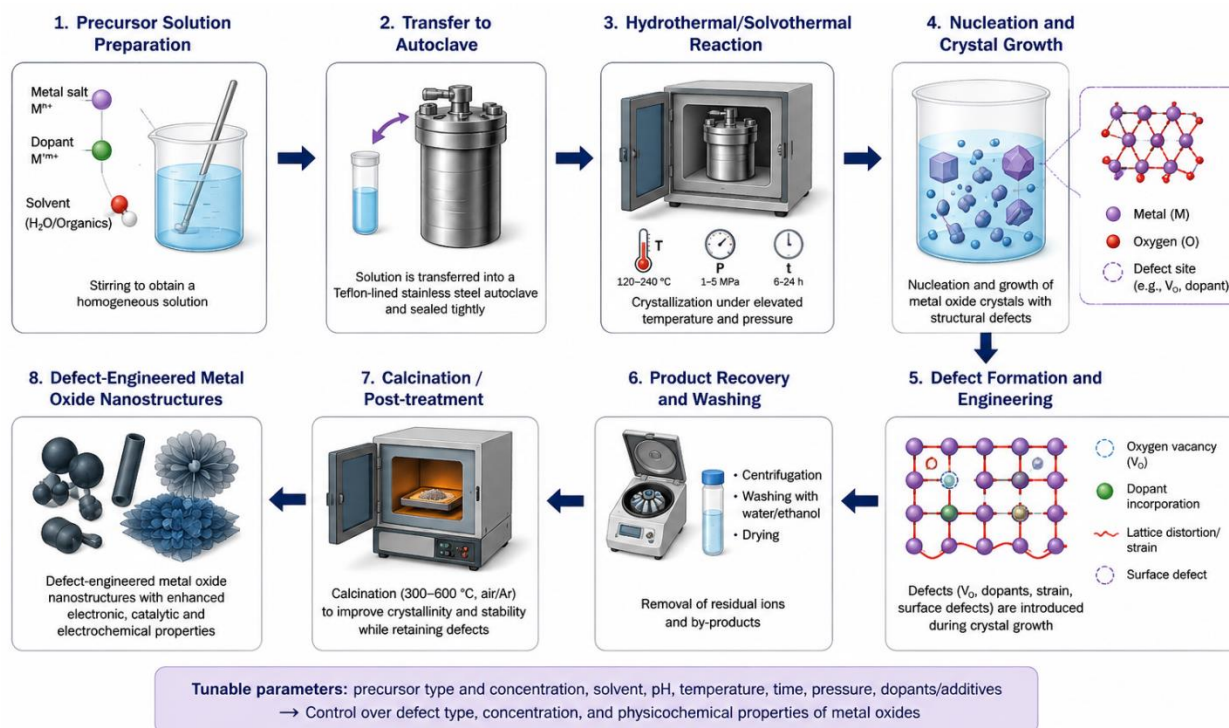


Fig. 6. Schematic illustration of the hydrothermal/solvothermal synthesis route for defect-engineered transition metal oxides.

CHEMICAL VAPOR DEPOSITION (CVD)

Chemical vapor deposition (CVD) is an advanced thin-film fabrication technique widely used for synthesizing high-purity defect-engineered metal oxide materials. In the CVD process, volatile precursor gases are introduced into a reaction chamber where they decompose or react at elevated temperatures to form solid thin films on a substrate surface. This method offers excellent control over film thickness, composition, crystallinity, and defect distribution. The controlled growth environment allows researchers to intentionally create oxygen vacancies and dopant-induced defects by modifying gas composition, deposition temperature, and reaction pressure. CVD-produced metal oxide films exhibit superior uniformity, strong adhesion, and high structural quality, making them suitable for electronic, optoelectronic, and sensing applications. Transition metal oxides synthesized through CVD, such as ZnO, SnO₂, and TiO₂, have demonstrated enhanced electrical conductivity, optical transparency, and catalytic performance due to controlled defect engineering. Despite its advantages, the CVD technique often requires expensive equipment and high operating temperatures, which may limit large-scale industrial applications. **Fig. 7** presents the sequential chemical vapor deposition process used to fabricate defect-engineered metal oxide thin films. Initially, volatile metal precursors, oxidizing gases, dopant sources, and carrier gases are supplied through controlled gas-delivery lines and mixed before entering the reaction chamber. Under elevated temperature and controlled pressure, the precursor species decompose or react on the heated substrate surface, resulting in the nucleation and growth of a uniform metal oxide thin film. By adjusting the precursor flow rate, oxygen-to-precursor ratio, substrate temperature, chamber pressure, deposition time, and dopant gas concentration, the concentration and distribution of oxygen vacancies, substitutional dopants, surface defects, and lattice strain can be precisely tailored. After deposition, controlled cooling and optional post-deposition annealing improve crystallinity, adhesion, and stability while preserving the desired defect structure. The final CVD-grown films exhibit high purity, uniform thickness, excellent adhesion, and enhanced electronic, optical, catalytic, and sensing properties.

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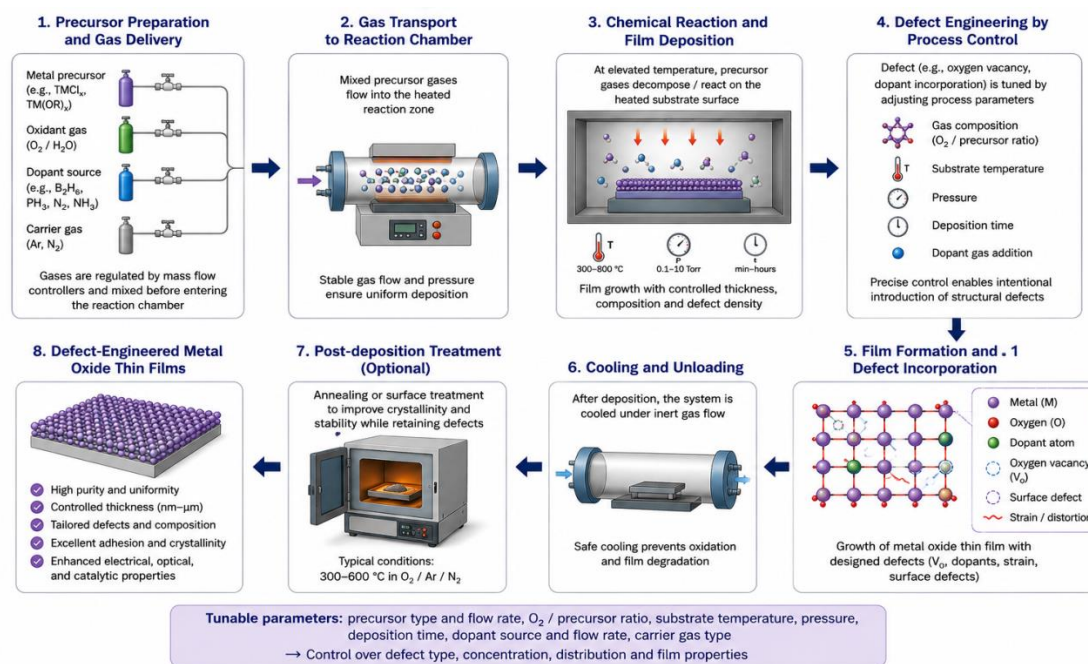


Fig. 7. Chemical vapor deposition (CVD) synthesis of defect-engineered metal oxide thin films.

ELECTROCHEMICAL SYNTHESIS

Electrochemical synthesis has emerged as an efficient and controllable approach for fabricating defect-engineered metal oxide materials. This technique involves electrochemical reactions occurring at electrode surfaces in an electrolyte solution under an applied electrical potential. By controlling parameters such as current density, electrolyte composition, applied voltage, and deposition time, researchers can tailor the morphology, oxidation state, and defect concentration of the synthesized materials. Electrochemical synthesis enables the formation of nanostructured metal oxides with high surface area and tunable electronic properties. Furthermore, this method allows precise control over oxygen vacancies and dopant incorporation, which significantly influence electrochemical performance. Electrochemically synthesized metal oxides are extensively investigated for applications in supercapacitors, lithium-ion batteries, fuel cells, and gas sensors. The method is considered environmentally friendly because it often operates under mild conditions and requires relatively low energy consumption compared to conventional thermal synthesis methods. Additionally, electrochemical synthesis provides excellent scalability and compatibility with flexible substrates for wearable electronic devices (see **Fig. 8**).

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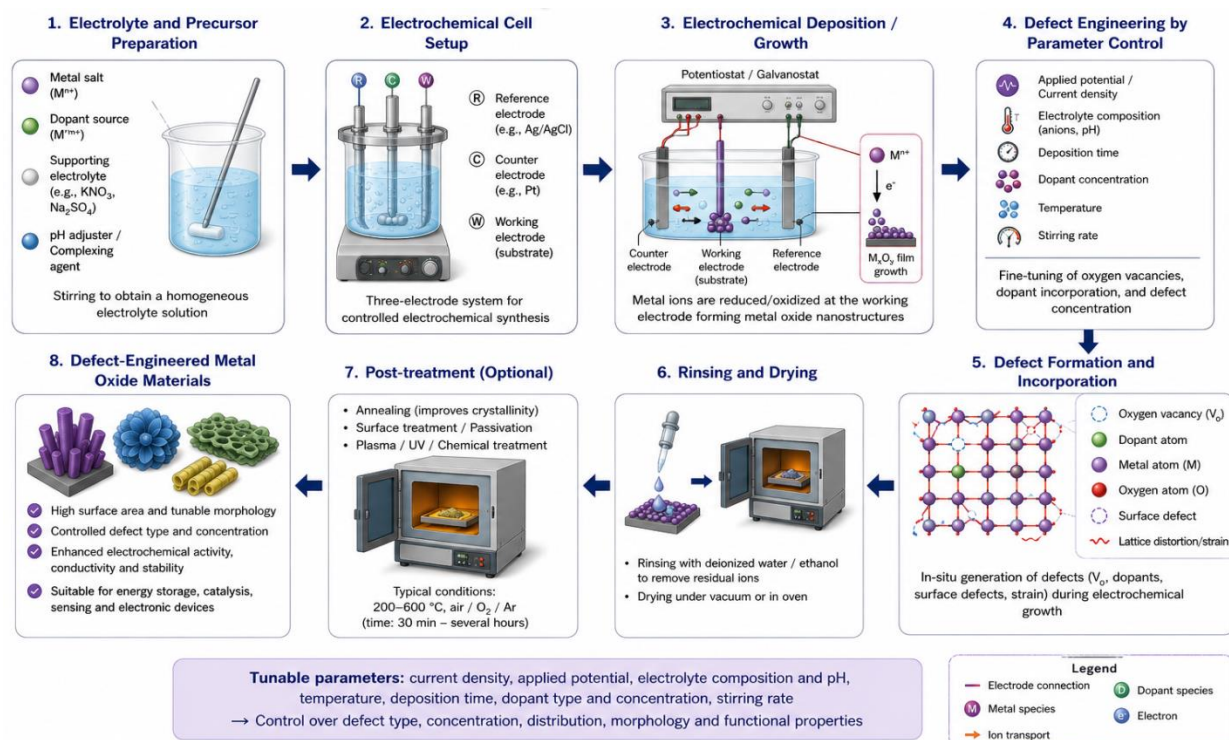


Fig. 8. Electrochemical synthesis of defect-engineered metal oxides.

GREEN SYNTHESIS APPROACHES

Green synthesis approaches have gained considerable attention as sustainable and environmentally friendly alternatives for producing defect-engineered metal oxide nanomaterials. Conventional synthesis methods often involve toxic chemicals, high energy consumption, and hazardous byproducts, which raise environmental and health concerns. In contrast, green synthesis utilizes natural resources such as plant extracts, microorganisms, biopolymers, and biodegradable solvents to reduce environmental impact. Plant extracts contain various phytochemicals, including flavonoids, alkaloids, and phenolic compounds, which can act as reducing and stabilizing agents during nanoparticle synthesis. Green synthesis methods offer several advantages, including low toxicity, cost-effectiveness, energy efficiency, and biocompatibility. Moreover, bio-assisted synthesis can influence defect formation and surface functionalization, thereby enhancing catalytic and antibacterial activities. Green-synthesized metal oxides such as ZnO, TiO₂, and Fe₂O₃ have demonstrated promising applications in environmental remediation, biomedical engineering, and photocatalysis. As sustainability becomes increasingly important in materials research, green synthesis approaches are expected to play a significant role in the future development of advanced nanomaterials (see Fig. 9).

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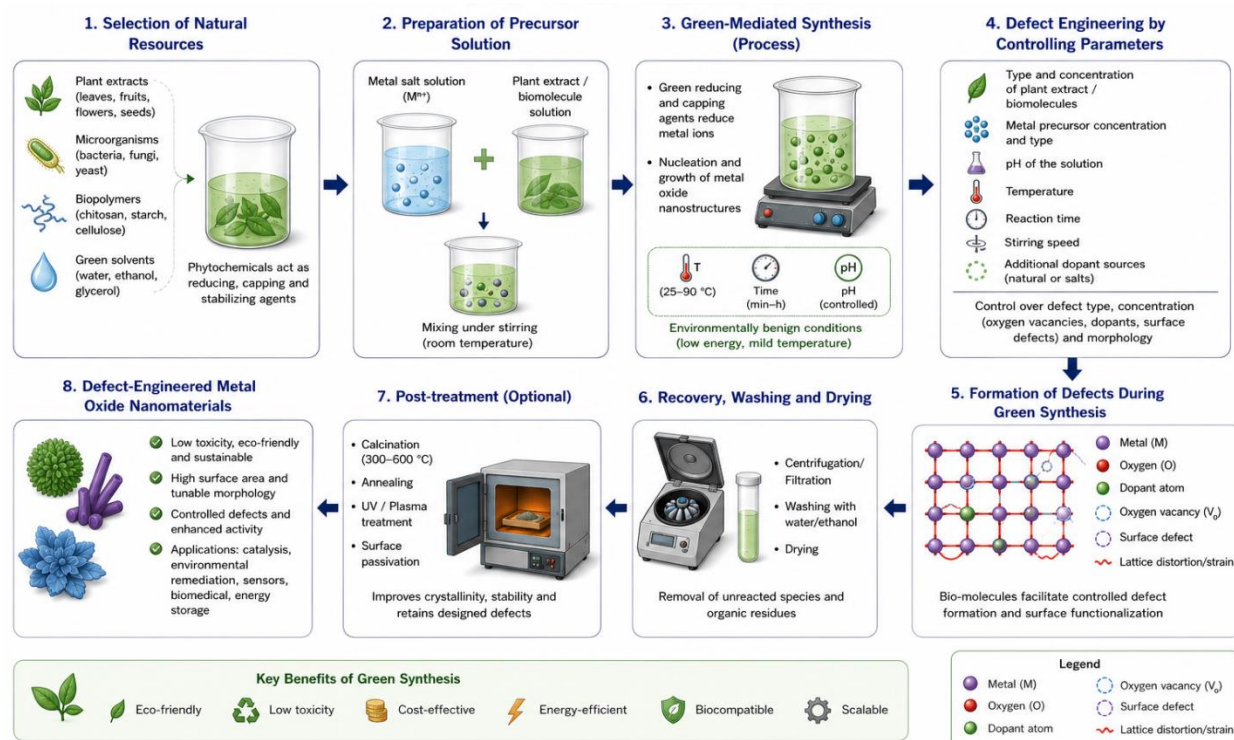


Fig. 9. Green synthesis of defect-engineered metal oxide nanomaterials

PARAMETERS AFFECTING DEFECT FORMATION

The formation and concentration of defects in transition metal oxides are strongly influenced by synthesis conditions and processing parameters. Careful control of these parameters is essential for optimizing material performance and achieving desired electronic, optical, and catalytic properties. Several important factors affecting defect formation include temperature, reaction atmosphere, dopants, and annealing conditions.

TEMPERATURE

Temperature is one of the most critical parameters affecting defect formation in metal oxides. Higher synthesis or calcination temperatures can promote crystal growth, phase transformation, and oxygen vacancy generation. Elevated temperatures increase atomic mobility within the crystal lattice, facilitating the formation and migration of defects. However, excessively high temperatures may also reduce surface area and lead to particle agglomeration, negatively affecting catalytic and electrochemical performance. Therefore, optimizing synthesis temperature is essential for balancing crystallinity and defect concentration.

ATMOSPHERE

The reaction atmosphere significantly influences the oxidation state and defect structure of metal oxides. Reducing atmospheres such as hydrogen or nitrogen can promote the formation of oxygen vacancies by removing oxygen atoms from the crystal lattice. In contrast, oxidizing atmospheres tend to suppress defect formation and stabilize higher oxidation states. Controlling the synthesis atmosphere is particularly important in tailoring electronic conductivity, catalytic activity, and gas sensing properties.

DOPANTS

Doping involves the intentional introduction of foreign atoms into the crystal structure of metal oxides to modify their electronic and structural properties. Dopants can alter charge balance, induce lattice distortion, and create additional defect states within the material. Rare-earth metals, transition metals, and non-metal elements are commonly used as dopants to improve conductivity, photocatalytic efficiency, and

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electrochemical performance. The type and concentration of dopants strongly influence defect density and overall material functionality.

ANNEALING CONDITIONS

Annealing treatment plays a vital role in controlling defect distribution, crystallinity, and phase stability in metal oxides. Parameters such as annealing temperature, duration, and atmosphere determine the formation and healing of defects within the crystal lattice. Controlled annealing can enhance oxygen vacancy concentration, improve crystallinity, and optimize charge transport properties. However, inappropriate annealing conditions may result in structural degradation or excessive defect recombination. Therefore, precise optimization of annealing parameters is essential for achieving high-performance defect-engineered metal oxide materials (see Fig. 10).

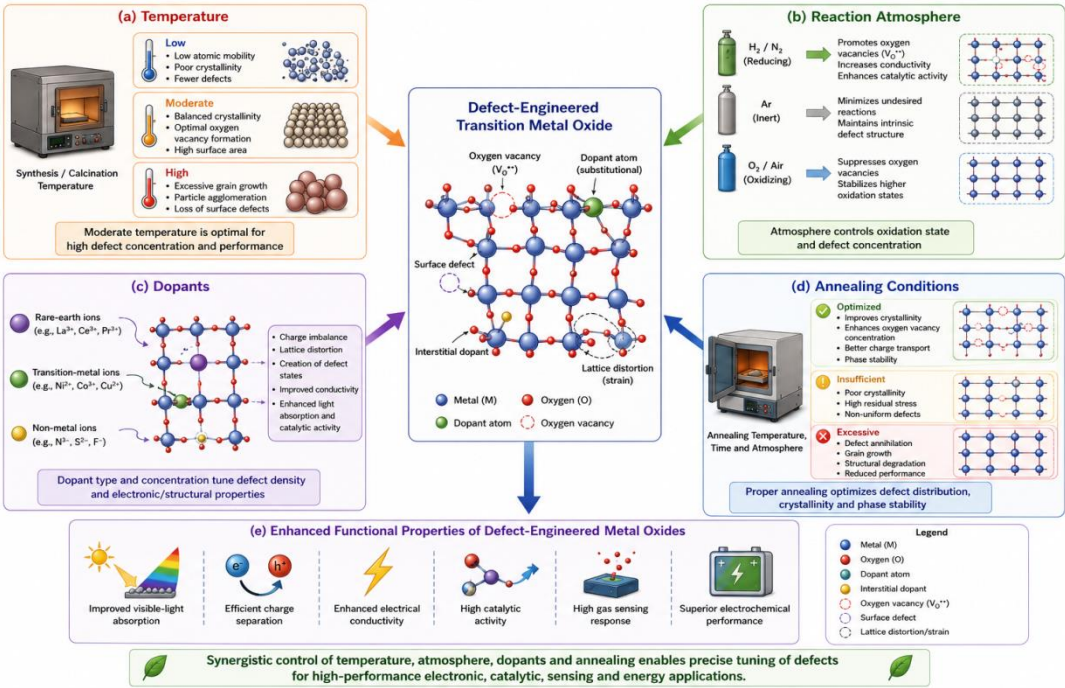


Fig. 10. Parameters affecting defect formation in transition metal oxides

DEFECT ENGINEERING STRATEGIES

Defect engineering is a powerful approach used to deliberately manipulate the atomic structure of transition metal oxides (TMOs) in order to improve their physical, chemical, electrical, optical, and catalytic properties. Unlike ideal crystals, real metal oxides contain various imperfections such as vacancies, interstitial atoms, substitutional dopants, grain boundaries, and lattice distortions. These defects significantly influence the electronic structure, charge carrier concentration, surface reactivity, and transport behavior of the materials. By carefully controlling the type, concentration, and distribution of defects, researchers can tailor the performance of TMOs for a wide range of applications, including photocatalysis, energy storage, gas sensing, electronics, and biomedical technologies. The most widely employed defect engineering strategies include oxygen vacancy engineering, elemental doping, surface modification, heterostructure formation, and strain engineering (see Fig. 11).

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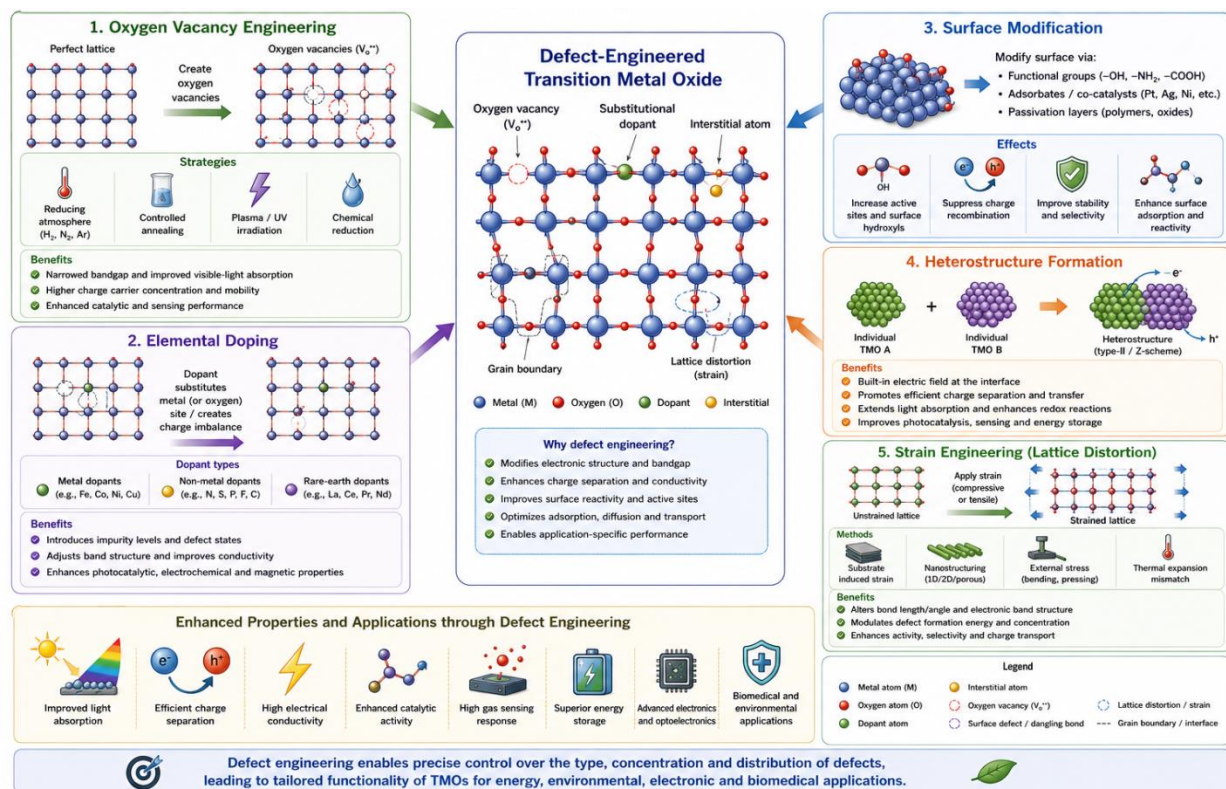


Fig. 11. Defect engineering strategies in transition metal

OXYGEN VACANCY ENGINEERING

Oxygen vacancy engineering is one of the most extensively studied defect engineering approaches in transition metal oxides. Oxygen vacancies are created when oxygen atoms are removed from their normal lattice positions, leaving empty sites within the crystal structure. These vacancies alter the local electronic environment by generating excess electrons that can participate in charge transport and surface reactions. The presence of oxygen vacancies often introduces defect states within the bandgap, thereby reducing the effective bandgap energy and extending light absorption into the visible region. Furthermore, oxygen vacancies can serve as active adsorption sites for reactant molecules such as oxygen, water, carbon dioxide, and toxic gases, enhancing catalytic and sensing performance. The creation of oxygen vacancies can be achieved through various techniques including thermal reduction, vacuum annealing, hydrogen treatment, plasma irradiation, laser processing, and chemical reduction methods. In photocatalytic applications, oxygen vacancies facilitate charge separation by trapping photogenerated electrons and suppressing electron-hole recombination. In energy storage devices, they improve ionic diffusion and electrical conductivity, while in gas sensors they enhance surface adsorption and sensitivity. Materials such as TiO_2 , ZnO , CeO_2 , WO_3 , and SnO_2 have demonstrated remarkable performance improvements after oxygen vacancy engineering, making this strategy one of the most effective methods for optimizing transition metal oxide properties (see Fig. 12).

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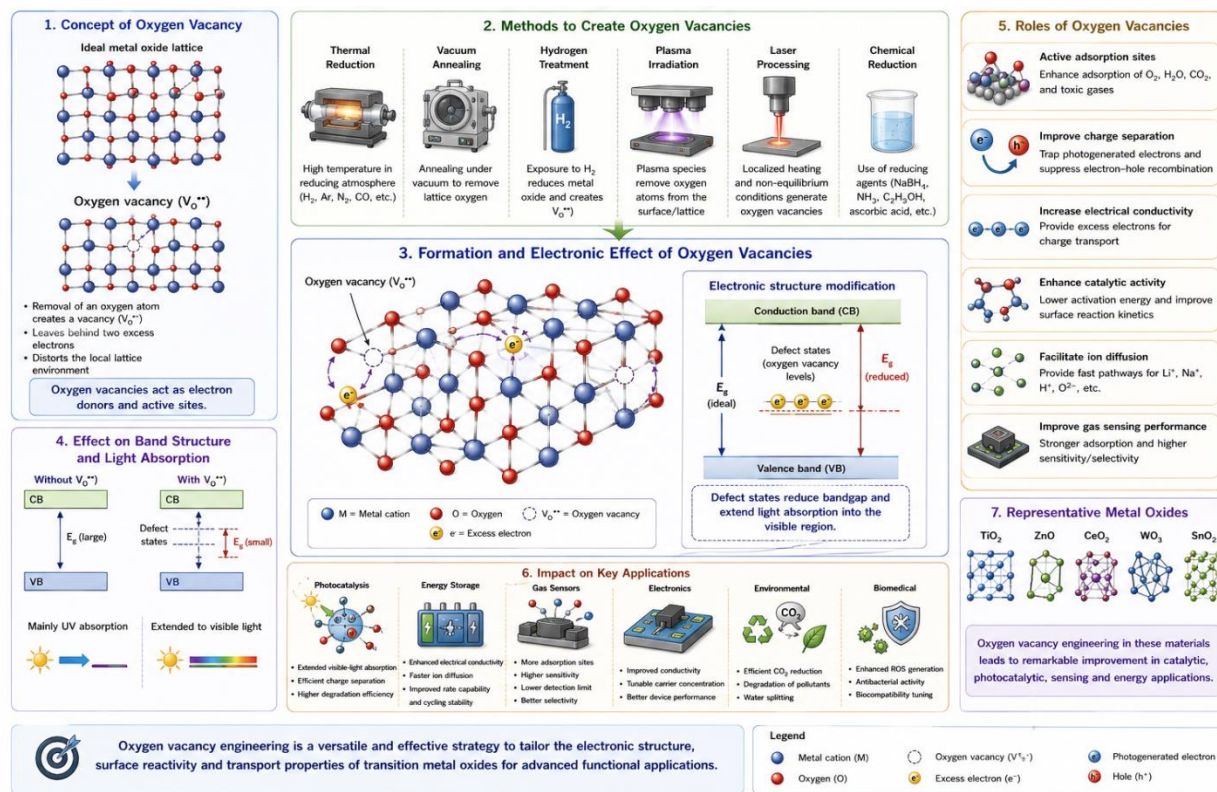


Fig. 12. Oxygen vacancy engineering in transition metal oxides, showing vacancy formation methods, electronic band-structure modification, enhanced light absorption and charge separation, and improved catalytic, sensing, and energy-storage performance.

ELEMENTAL DOPING

Elemental doping involves the intentional incorporation of foreign atoms into the crystal lattice of metal oxides to modify their structural and electronic characteristics. Dopants may substitute host metal ions or occupy interstitial lattice positions, creating localized electronic states and influencing defect formation. Doping can significantly alter the band structure, carrier concentration, conductivity, optical absorption, and catalytic activity of metal oxides. In many cases, dopants promote the formation of oxygen vacancies, resulting in synergistic effects that further enhance material performance. The effectiveness of doping depends on factors such as dopant type, concentration, ionic radius, valence state, and distribution within the host lattice. Properly selected dopants can improve charge separation, expand visible-light absorption, increase active surface sites, and stabilize crystal structures. Depending on the nature of the dopant, elemental doping is commonly categorized into rare earth doping, non-metal doping, and transition metal doping (see **Fig. 13**).

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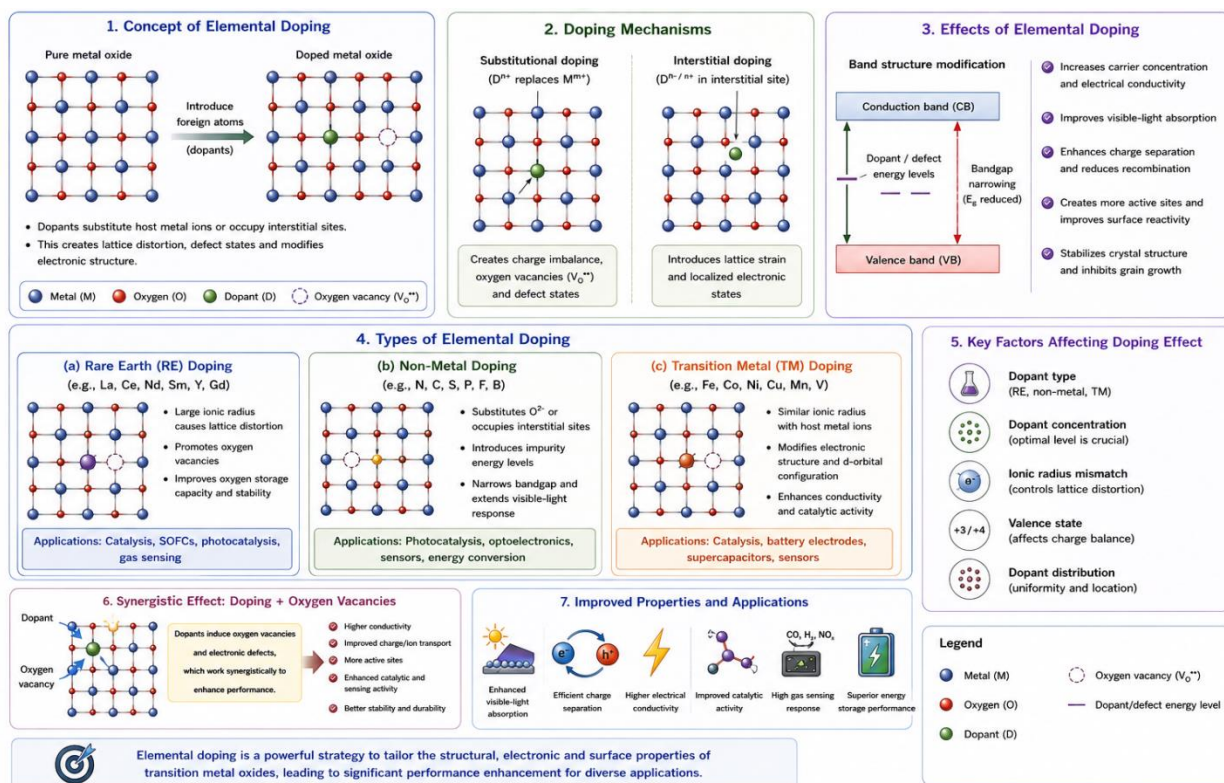


Fig. 13. Elemental doping in transition metal oxides

RARE EARTH DOPING

Rare earth doping has attracted significant interest because rare earth elements possess unique electronic configurations characterized by partially filled 4f orbitals. When rare earth ions such as lanthanum (La), cerium (Ce), neodymium (Nd), samarium (Sm), europium (Eu), and gadolinium (Gd) are incorporated into metal oxide lattices, they introduce localized energy states that can improve charge separation and light absorption. The difference in ionic size and valence between rare earth ions and host cations often generates lattice distortions and promotes oxygen vacancy formation. Rare earth dopants enhance photocatalytic activity by increasing visible-light absorption and suppressing electron-hole recombination. They also improve thermal stability, inhibit grain growth, and increase specific surface area. For example, Ce-doped TiO_2 exhibits improved visible-light photocatalytic performance, while La-doped ZnO demonstrates enhanced gas sensing capabilities. In cerium oxide-based materials, rare earth doping can significantly improve oxygen storage capacity and redox behavior. Consequently, rare earth doping is widely employed in photocatalysis, fuel cells, sensors, and environmental remediation technologies (see **Fig. 14**).

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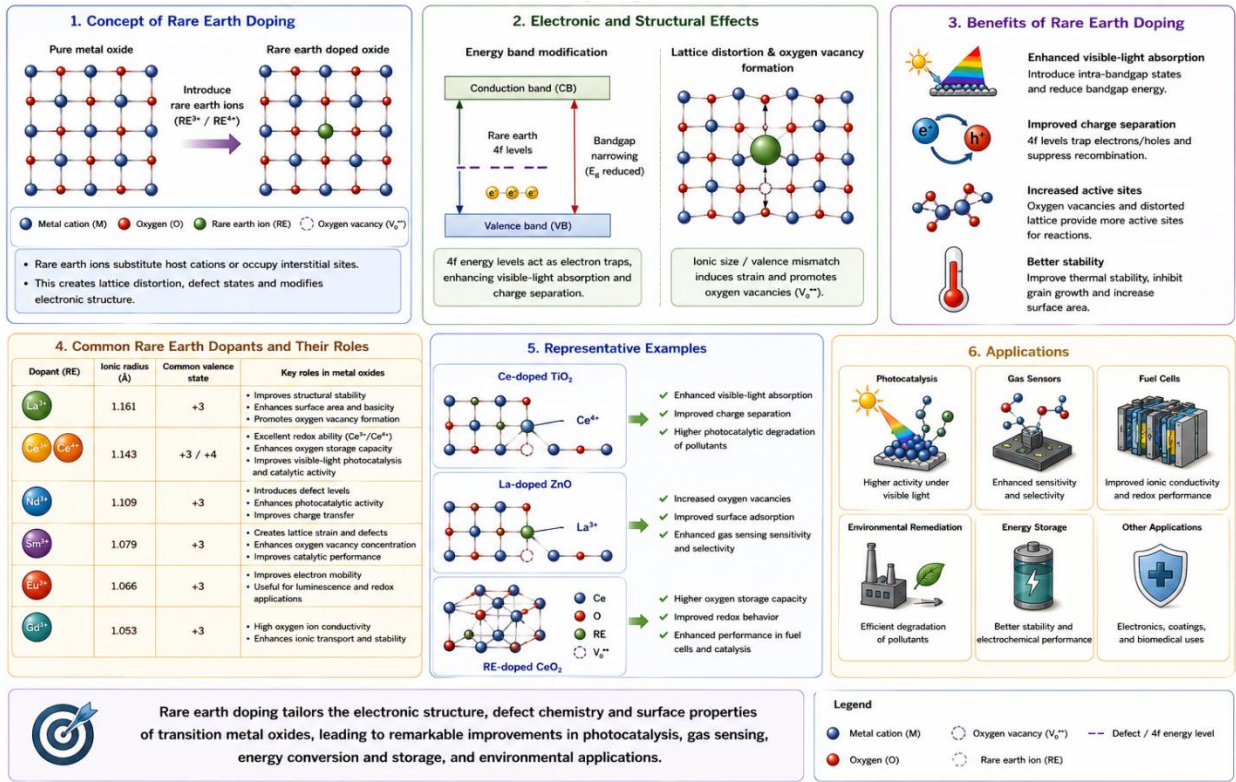


Fig. 14. Rare earth doping in transition metal oxides

NON-METAL DOPING

Non-metal doping involves the incorporation of elements such as nitrogen, carbon, sulfur, phosphorus, boron, and fluorine into the crystal lattice of metal oxides. Unlike metal dopants, non-metal dopants primarily influence the valence band structure through orbital hybridization with oxygen atoms. This interaction can narrow the bandgap and extend optical absorption into the visible-light region, thereby enhancing solar energy utilization. Nitrogen-doped TiO_2 is one of the most studied examples of non-metal doping, where nitrogen introduces impurity levels above the valence band, enabling visible-light photocatalysis. Similarly, sulfur and carbon doping improve the photocatalytic efficiency of ZnO and CeO_2 by enhancing light harvesting and charge transport. Non-metal dopants can also create surface defects and modify adsorption behavior, which is beneficial for catalytic reactions and pollutant degradation. Due to their ability to improve optical properties without significantly compromising structural stability, non-metal dopants are widely utilized in photocatalysts, sensors, and optoelectronic devices (see Fig. 15).

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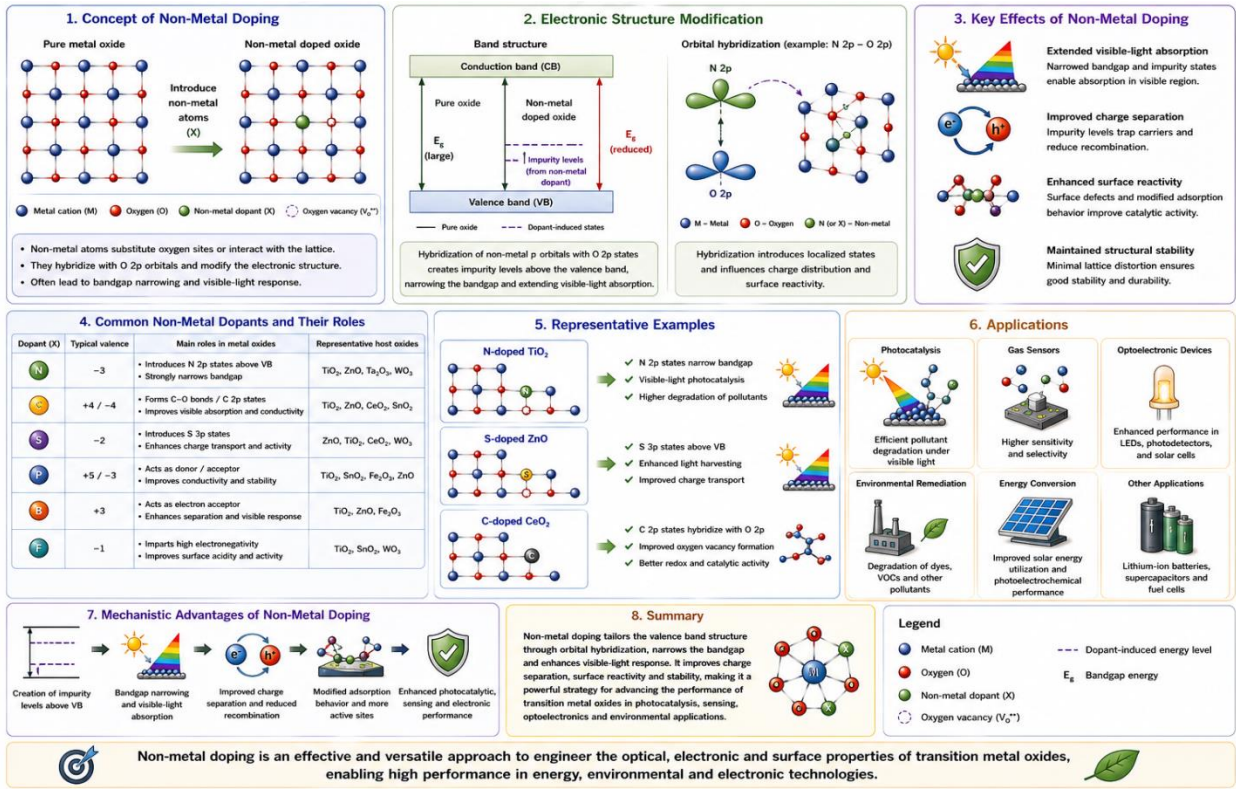


Fig. 15. Non-metal doping in transition metal oxides

TRANSITION METAL DOPING

Transition metal doping is a highly effective strategy for modifying the electronic, magnetic, and catalytic properties of metal oxides. Transition metal ions such as Fe, Co, Ni, Mn, Cu, Cr, and V possess partially filled d orbitals that introduce additional energy levels within the band structure of the host material. These dopants can increase carrier concentration, improve electrical conductivity, and enhance catalytic activity through the formation of new active reaction centers. The incorporation of transition metal ions often results in synergistic interactions with oxygen vacancies, leading to enhanced charge transfer and improved catalytic performance. For example, Fe-doped TiO₂ exhibits stronger visible-light absorption and higher photocatalytic activity than undoped TiO₂. Similarly, Co-doped ZnO shows improved gas sensing characteristics, while Ni-doped CeO₂ demonstrates enhanced redox behavior and catalytic efficiency. In addition to photocatalysis and sensing applications, transition metal doping is widely used in magnetic materials, energy storage devices, and spintronic technologies (see Fig. 16).

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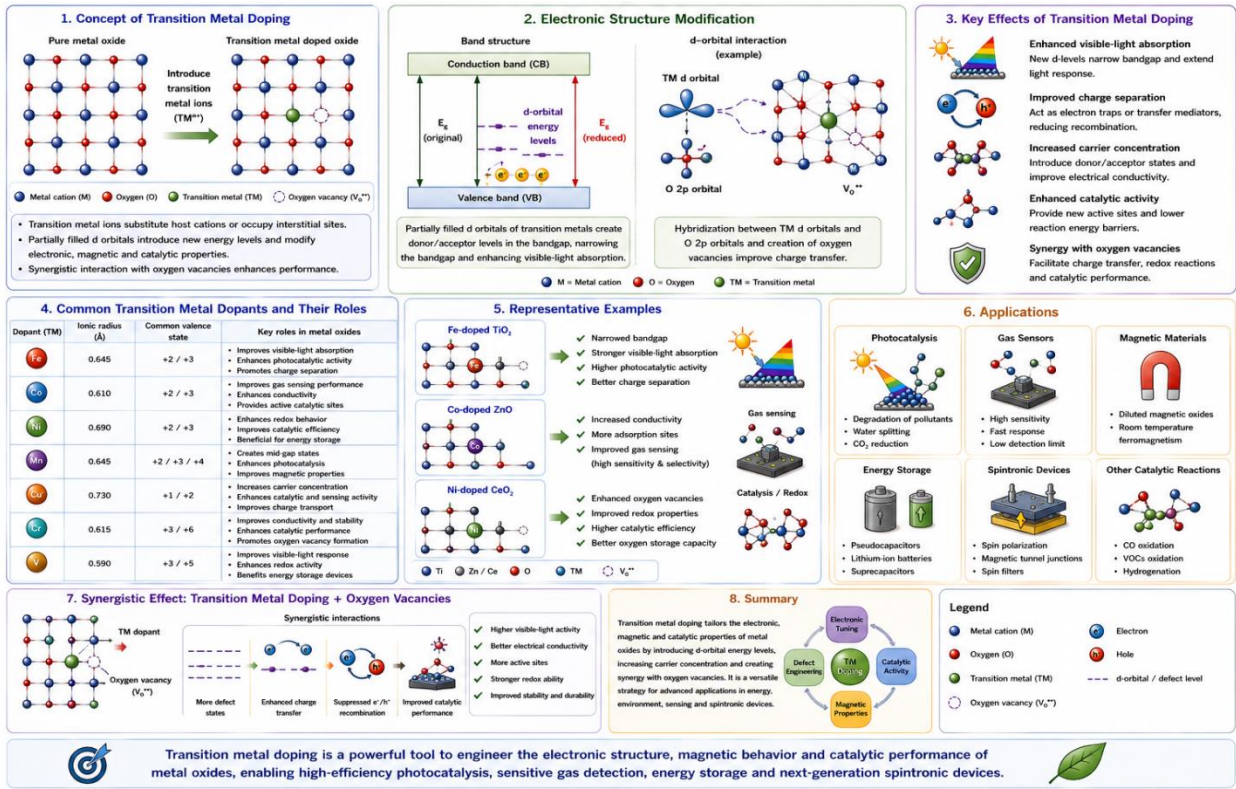


Fig. 16. Transition metal doping in transition metal oxides

SURFACE MODIFICATION

Surface modification focuses on tailoring the outermost atomic layers of metal oxide materials to improve their interaction with surrounding environments. Since most catalytic, sensing, and biological processes occur at the surface, modifying surface characteristics can significantly enhance overall performance. Surface modification techniques include plasma treatment, chemical functionalization, noble metal decoration, polymer coating, and surface etching. The introduction of surface defects and functional groups increases the number of active reaction sites and improves molecular adsorption. Noble metal nanoparticles such as platinum, gold, and silver can serve as electron sinks that facilitate charge separation and transfer. Surface modification also enhances corrosion resistance, chemical stability, and biocompatibility. For example, platinum-decorated TiO_2 exhibits superior photocatalytic hydrogen production, while silver-coated ZnO nanoparticles demonstrate enhanced antibacterial activity. Therefore, surface engineering plays a critical role in maximizing the functionality of defect-engineered metal oxides (see Fig. 17).

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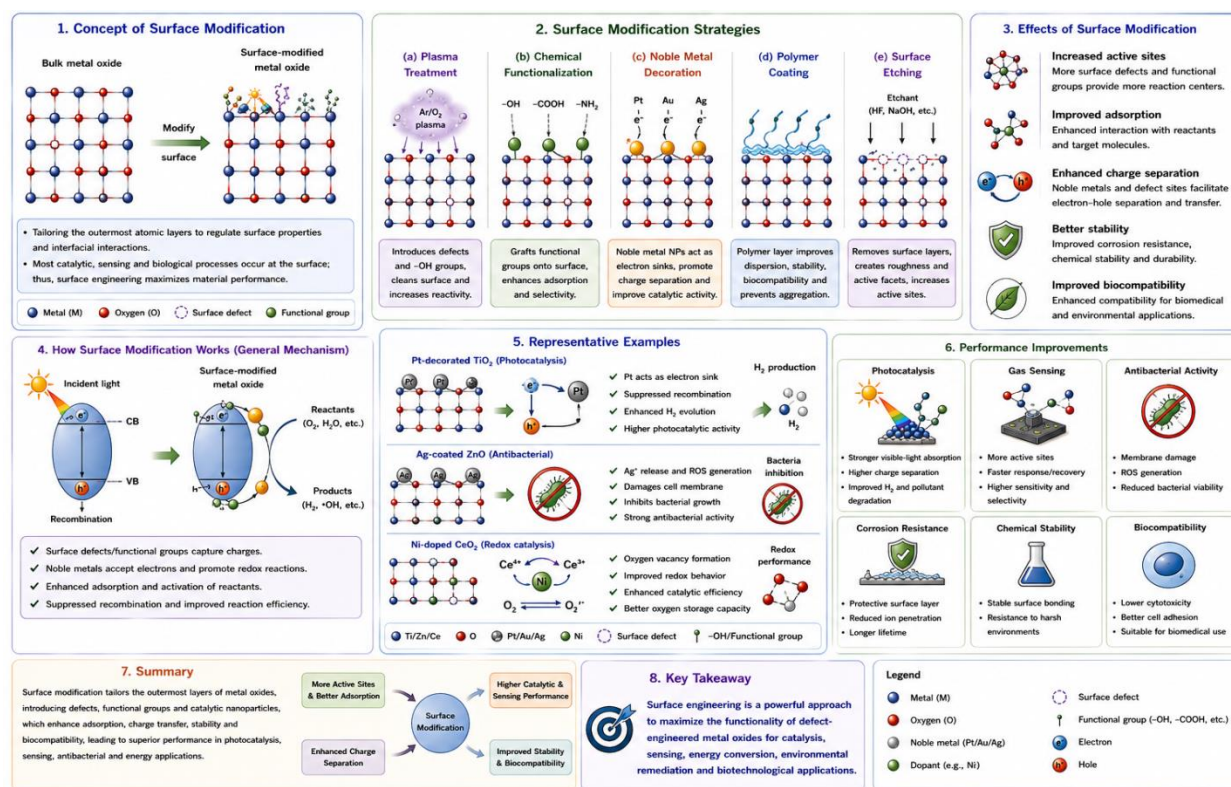


Fig. 17. Surface modification of defect-engineered transition metal oxides

HETEROSTRUCTURE FORMATION

Heterostructure formation involves combining two or more semiconductor materials with different electronic properties to create interfaces that promote efficient charge transfer. In transition metal oxide systems, heterostructures are widely employed to overcome the limitations of individual materials, such as rapid electron-hole recombination and narrow spectral response. The interfaces formed between different materials generate internal electric fields that facilitate charge separation and transport. Various heterojunction architectures, including type-I, type-II, Z-scheme, and S-scheme systems, have been developed to optimize photocatalytic and electronic performance. For example, TiO₂/ZnO heterostructures exhibit enhanced photocatalytic efficiency due to improved charge separation, while CeO₂/TiO₂ composites benefit from synergistic redox interactions. The formation of heterostructures also broadens light absorption and increases the number of catalytic active sites. As a result, heterostructure engineering has become a fundamental strategy for designing high-performance photocatalysts, sensors, and energy conversion devices (see **Fig. 18**).

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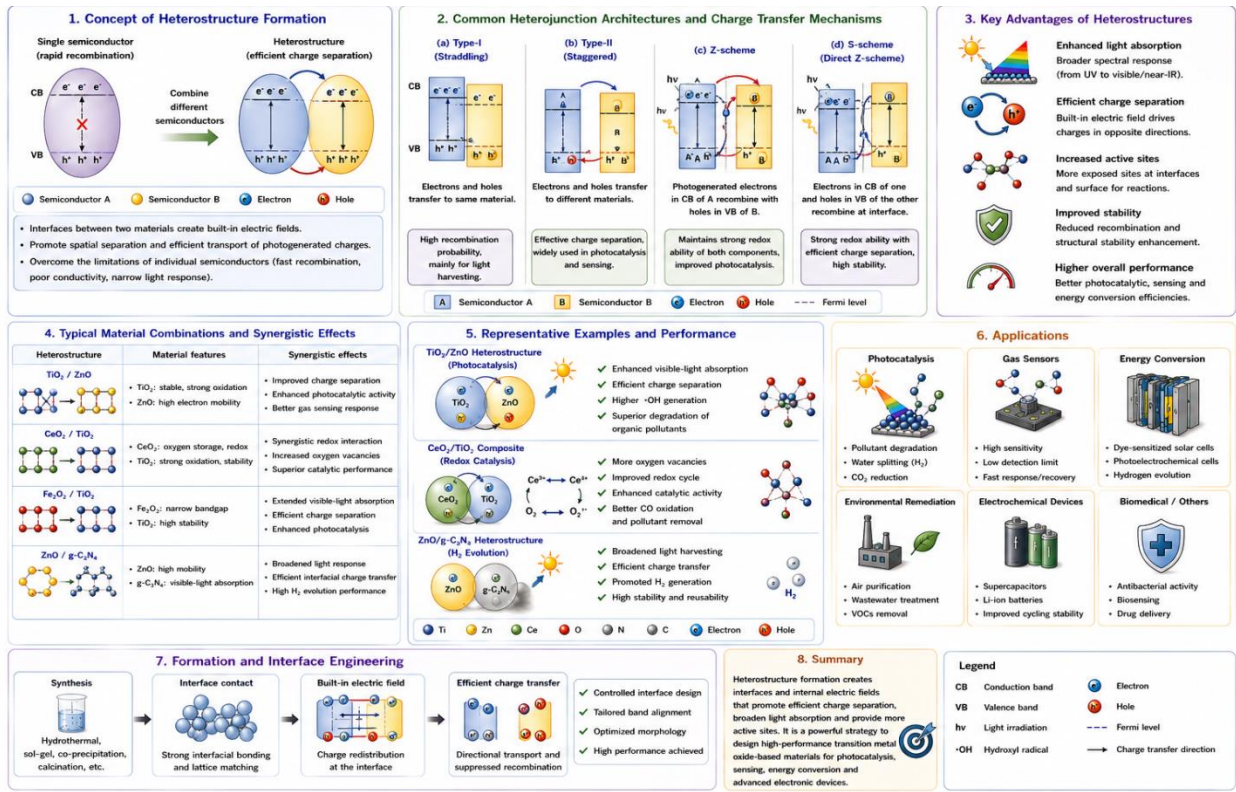


Fig. 18. Hetrostructure formation in transition metal oxides

STRAIN ENGINEERING

Strain engineering refers to the deliberate manipulation of lattice distortions within a material to modify its electronic and structural properties. Strain can be introduced through lattice mismatch in thin films, thermal expansion differences, mechanical deformation, or epitaxial growth techniques. These distortions alter bond lengths and bond angles, thereby affecting the electronic band structure and defect formation energies. The application of strain can significantly influence carrier mobility, conductivity, optical absorption, and catalytic activity. In many cases, strained lattices promote the formation of oxygen vacancies and other beneficial defects. Strain-induced modifications can also optimize adsorption energies for reactant molecules, leading to enhanced catalytic performance. Examples include strained TiO₂ thin films, ZnO nanowires, and CeO₂ epitaxial layers, which exhibit improved photocatalytic activity and charge transport properties. As advanced fabrication technologies continue to evolve, strain engineering is expected to play an increasingly important role in next-generation functional materials (see Fig. 19).

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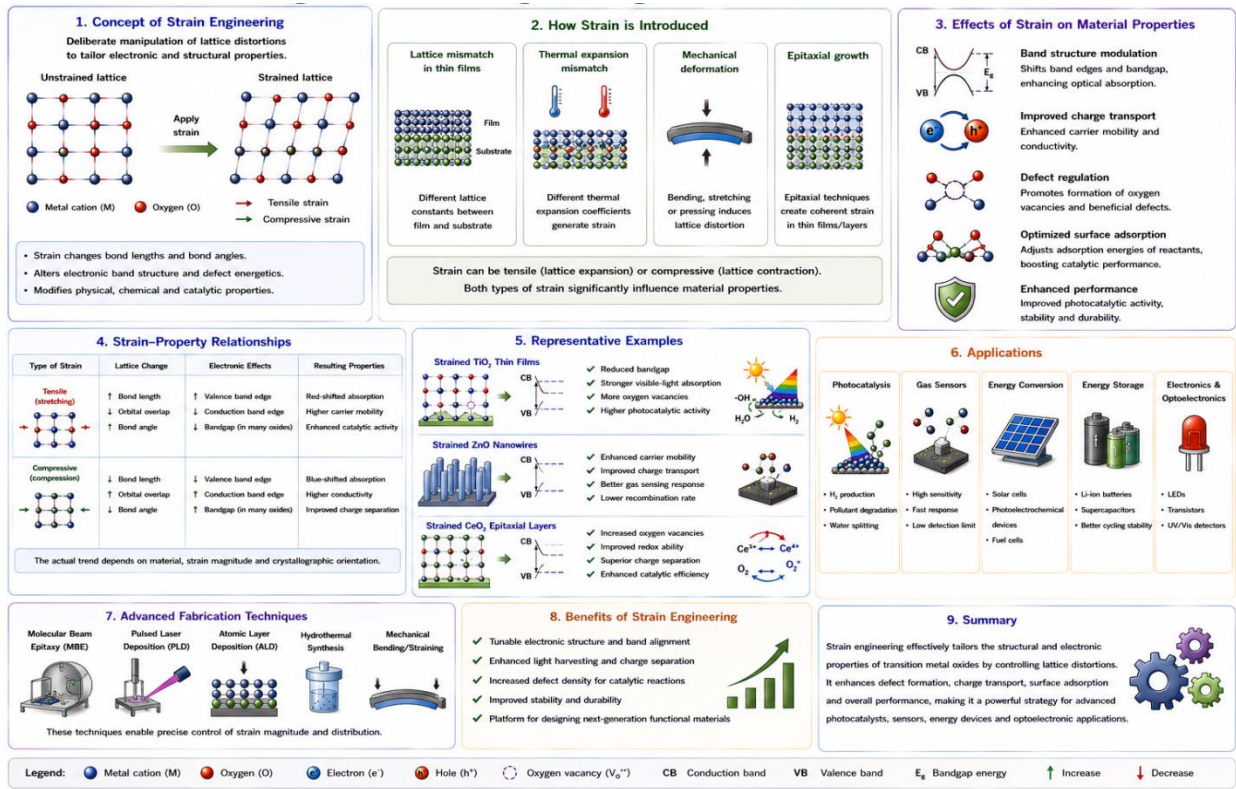


Fig. 19. Strain engineering in transition metal oxides

APPLICATIONS OF DEFECT-ENGINEERED METAL OXIDES

Defect engineering has emerged as a powerful tool for enhancing the performance of transition metal oxides in numerous technological applications. By introducing controlled defects such as oxygen vacancies, dopants, lattice distortions, and interfacial structures, researchers can significantly improve charge transport, catalytic activity, optical absorption, ion diffusion, and surface reactivity. These improvements have enabled defect-engineered metal oxides to play a central role in energy conversion, energy storage, environmental remediation, sensing technologies, electronic devices, and biomedical systems. The versatility of defect engineering makes it one of the most important approaches for developing advanced multifunctional materials.

PHOTOCATALYSIS

Photocatalysis is one of the most extensively studied applications of defect-engineered metal oxides. In a photocatalytic process, semiconductor materials absorb photons with energies equal to or greater than their bandgap, generating electron-hole pairs that participate in redox reactions on the material surface. However, conventional photocatalysts often suffer from limited visible-light absorption and rapid recombination of photogenerated charge carriers. Defect engineering addresses these limitations by introducing intermediate energy levels, enhancing charge separation, and increasing the number of active reaction sites. As a result, defect-rich metal oxides exhibit significantly improved photocatalytic efficiency for hydrogen production, pollutant degradation, and carbon dioxide conversion (see Fig. 20).

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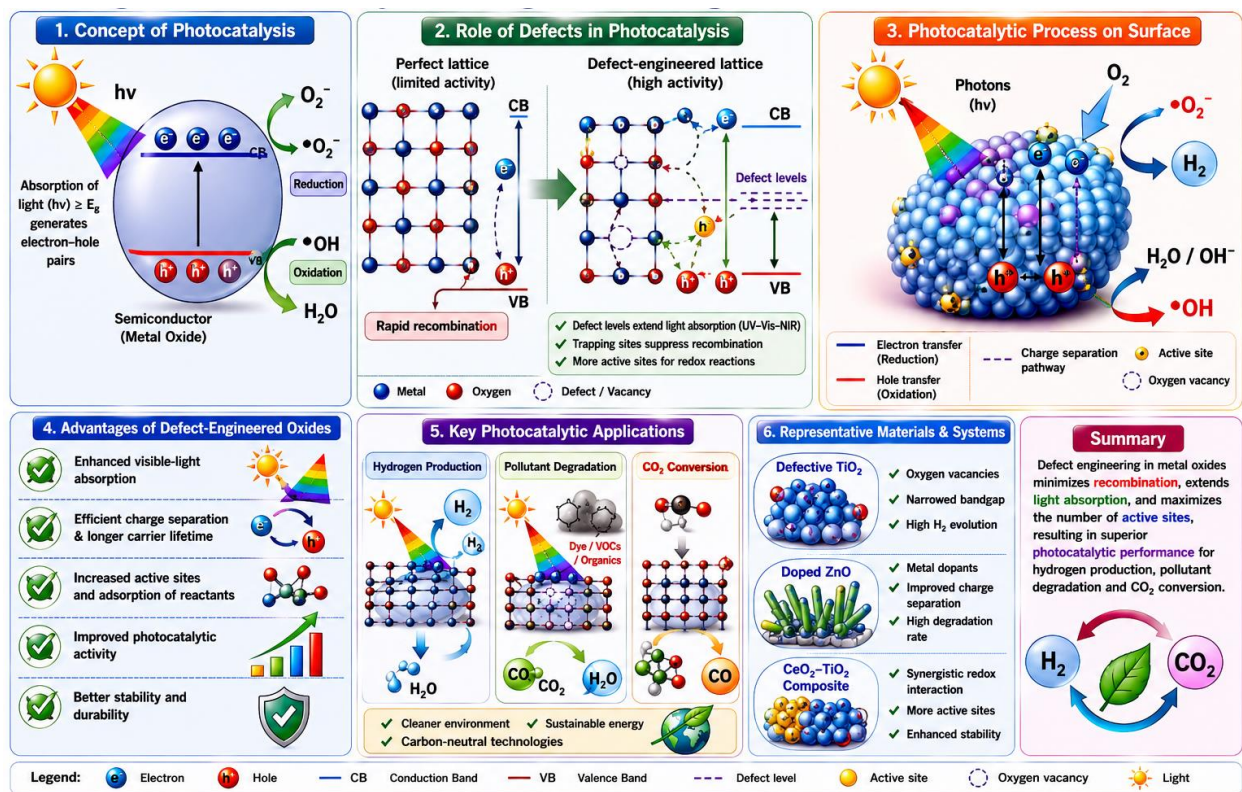


Fig. 20. Photocatalytic mechanism of defect-engineered transition metal oxides, showing enhanced light absorption, charge separation, surface redox reactions, and applications in hydrogen production, pollutant degradation, and CO₂ conversion.

WATER SPLITTING

Photocatalytic water splitting represents a sustainable approach for producing hydrogen fuel using solar energy. The process involves the decomposition of water molecules into hydrogen and oxygen through photocatalytic reactions. Efficient water splitting requires effective light absorption, rapid charge separation, and sufficient catalytic activity for hydrogen evolution and oxygen evolution reactions. Defects such as oxygen vacancies provide active adsorption sites for water molecules and facilitate charge transfer processes. These vacancies also introduce defect states within the bandgap, enabling enhanced visible-light absorption. Materials such as oxygen-deficient TiO₂, defective WO₃, and vacancy-rich CeO₂ have demonstrated remarkable improvements in hydrogen production rates compared with their pristine counterparts. The presence of defects promotes electron mobility and suppresses electron-hole recombination, thereby increasing photocatalytic efficiency. Consequently, defect engineering is considered a key strategy for advancing solar hydrogen production technologies and supporting the transition toward clean and renewable energy systems (see Fig. 21).

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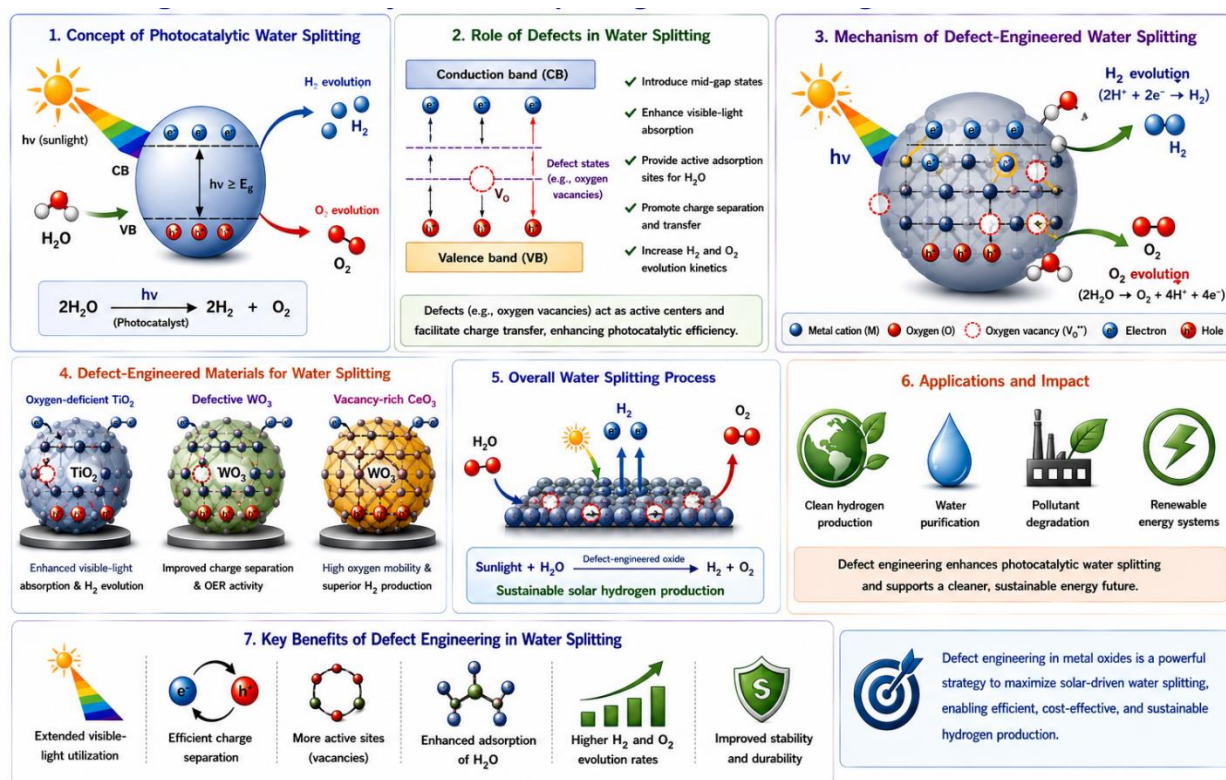


Fig. 21. Photocatalytic water splitting using defect-engineered metal oxides, showing enhanced light absorption, charge separation, water adsorption, and hydrogen and oxygen evolution

DYE DEGRADATION

The degradation of organic dyes is an important environmental application of photocatalysis, particularly for wastewater treatment. Industrial dyes such as methylene blue, rhodamine B, methyl orange, and congo red are persistent pollutants that pose serious environmental and health risks. Defect-engineered metal oxides can effectively degrade these pollutants through the generation of highly reactive oxygen species, including hydroxyl radicals and superoxide radicals. Oxygen vacancies and dopant-induced defects increase the adsorption capacity of photocatalysts and improve the separation of photogenerated charge carriers. These effects enhance the production of reactive species responsible for breaking down complex organic molecules into harmless products such as carbon dioxide and water. Defective TiO_2 , ZnO , CeO_2 , and WO_3 photocatalysts have shown significantly higher degradation efficiencies than defect-free materials. As environmental regulations become increasingly stringent, defect-engineered photocatalysts are expected to play a critical role in sustainable wastewater purification technologies (see **Fig. 22**).

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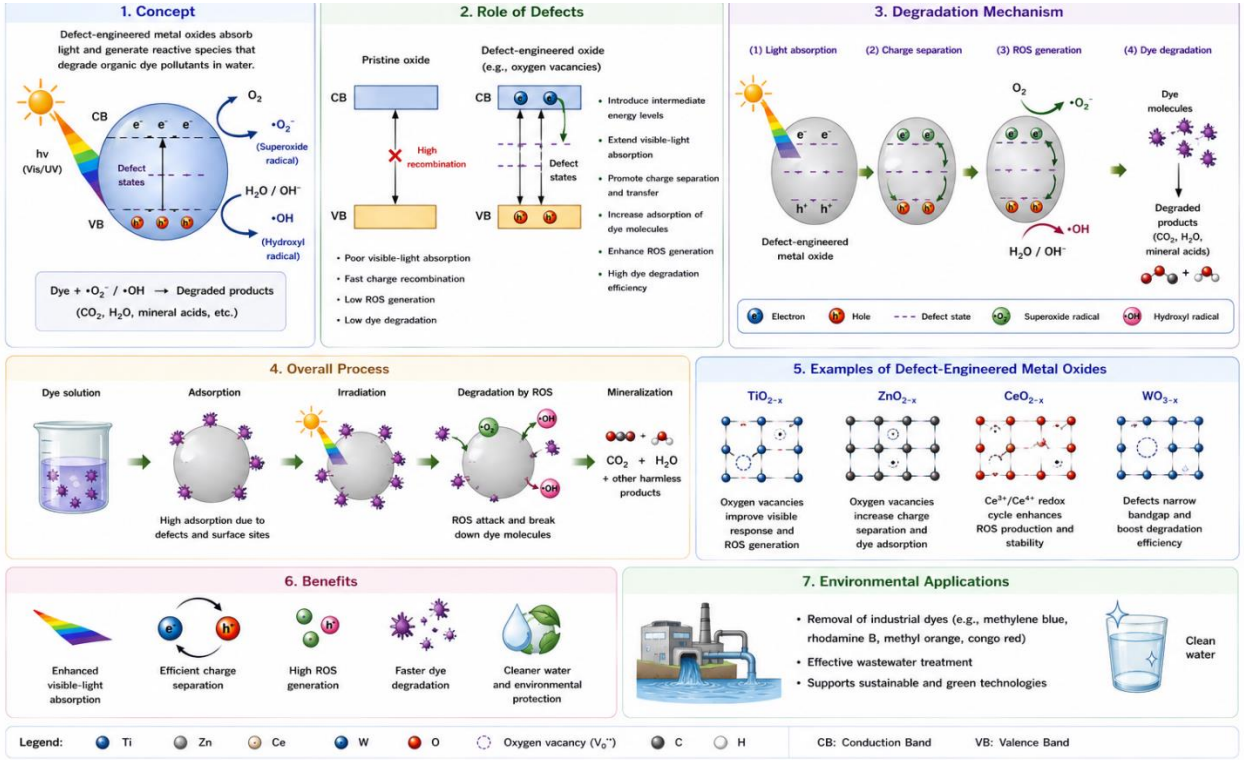


Fig. 22. Photocatalytic degradation of organic dyes by defect-engineered metal oxides through enhanced light absorption, charge separation, reactive oxygen species generation, and conversion of dye pollutants into harmless products.

CO2 REDUCTION

Photocatalytic carbon dioxide reduction has attracted considerable attention as a promising approach for mitigating greenhouse gas emissions while simultaneously producing valuable fuels and chemicals. Carbon dioxide is a highly stable molecule that requires substantial activation energy to undergo chemical conversion. Defects within metal oxides provide active adsorption sites that facilitate CO₂ activation and lower reaction energy barriers. Oxygen vacancies are particularly effective in promoting carbon dioxide adsorption because they create electron-rich regions capable of interacting strongly with CO₂ molecules. These defect sites enable the transfer of photogenerated electrons to adsorbed carbon dioxide, leading to the formation of products such as carbon monoxide, methane, methanol, and formic acid. Defect-engineered TiO₂, CeO₂, ZnO, and WO₃ have demonstrated enhanced CO₂ reduction performance due to improved light absorption and charge transfer characteristics. The continued development of defect-rich photocatalysts could contribute significantly to carbon-neutral energy technologies and sustainable chemical production (see Fig. 23).

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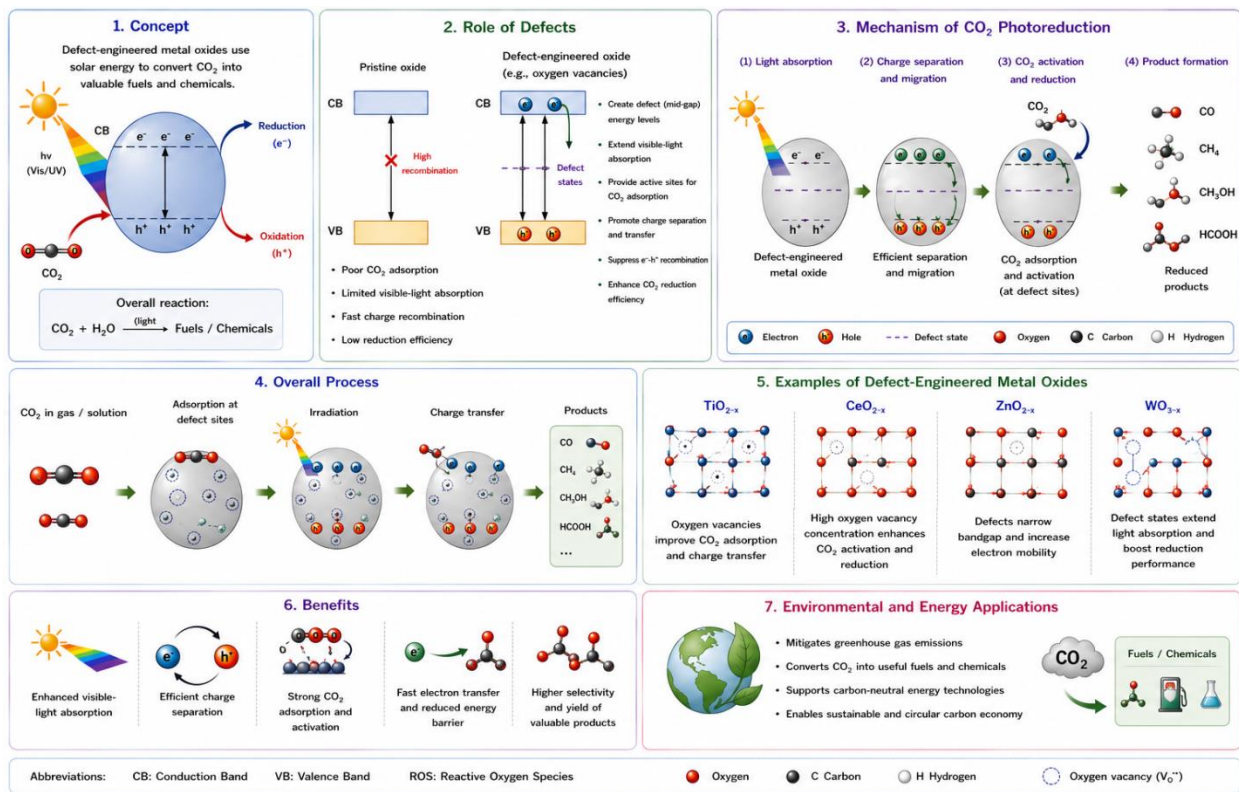


Fig. 23. Photocatalytic CO₂ reduction using defect-engineered metal oxides, showing enhanced CO₂ adsorption, charge transfer, and conversion into valuable fuels and chemicals

ENERGY STORAGE

The growing demand for portable electronics, electric vehicles, and renewable energy systems has increased the need for high-performance energy storage devices. Defect engineering provides an effective means of improving the electrochemical properties of metal oxide electrodes by enhancing conductivity, increasing active storage sites, and facilitating ion transport. Through careful defect control, researchers can optimize battery and supercapacitor performance, achieving higher energy density, faster charging rates, and longer cycle life (see **Fig. 24**).

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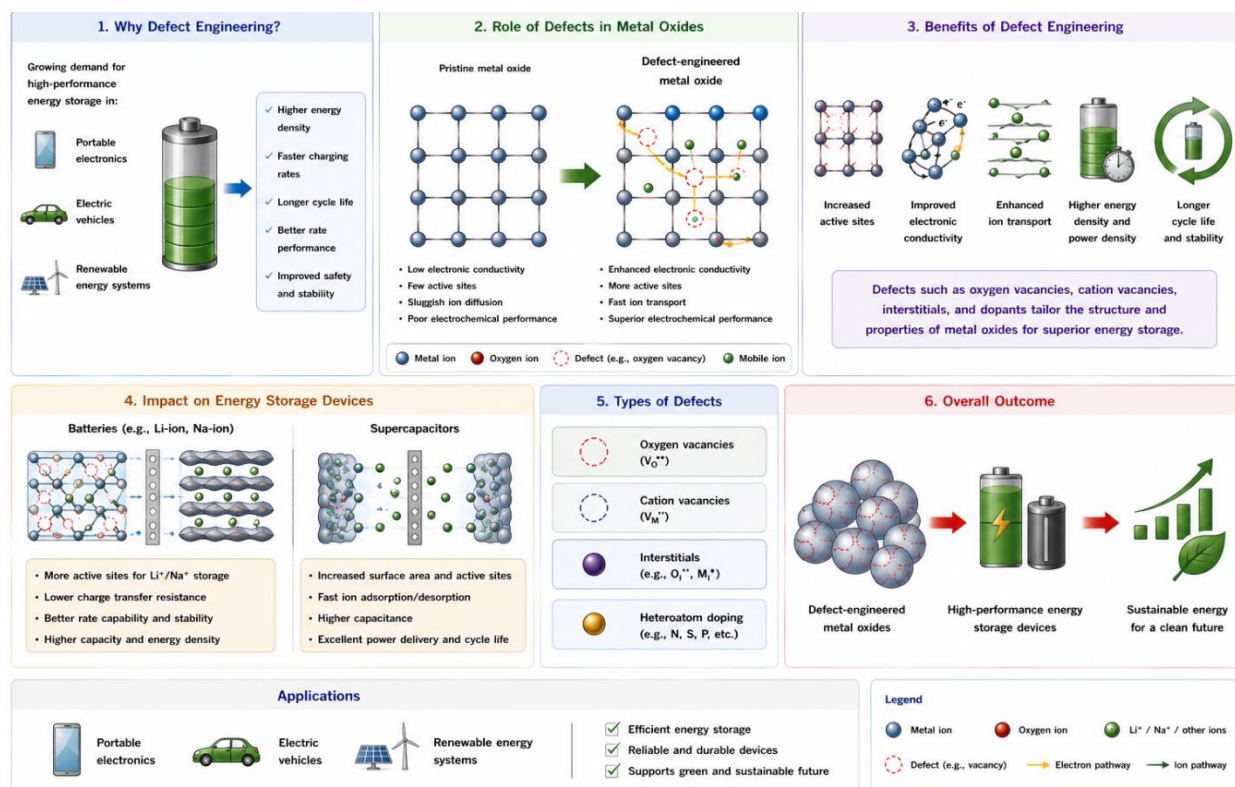


Fig. 24. Energy-storage enhancement in defect-engineered metal oxides, showing improved conductivity, ion transport, active-site density, capacity, rate capability, and cycling stability for batteries and supercapacitors.

LITHIUM-ION BATTERIES

Lithium-ion batteries are currently the dominant energy storage technology due to their high energy density and long cycle life. However, many metal oxide electrode materials suffer from poor conductivity and limited lithium-ion diffusion rates. Defect engineering addresses these challenges by introducing oxygen vacancies, dopants, and lattice distortions that facilitate electron transport and ion migration. Oxygen vacancies create additional lithium storage sites and reduce diffusion barriers, enabling faster charge-discharge processes. Furthermore, defect-induced electronic states enhance electrical conductivity and improve overall electrode kinetics. Defective TiO_2 , Fe_2O_3 , MnO_2 , and Co_3O_4 have demonstrated significantly improved specific capacities, rate capabilities, and cycling stability compared with pristine materials. As battery technologies continue to evolve, defect engineering is expected to play a central role in the development of next-generation lithium-ion batteries with superior performance characteristics (see Fig. 25).

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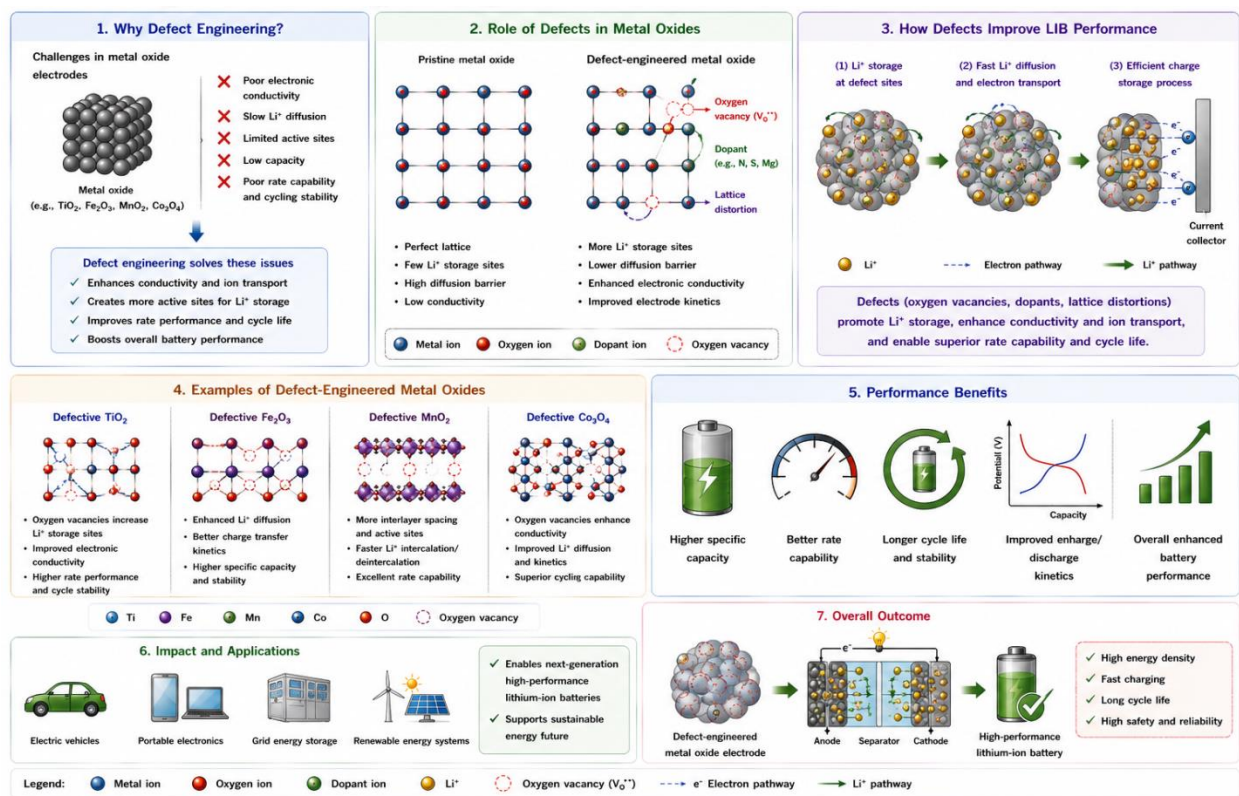


Fig. 25. Defect engineering in metal oxide electrodes for lithium-ion batteries, showing improved lithium-ion storage, electron transport, rate capability, specific capacity, and cycling stability.

SUPERCAPACITORS

Supercapacitors are energy storage devices characterized by high power density, rapid charging capability, and excellent cycling stability. The performance of supercapacitors depends strongly on the surface area, conductivity, and availability of electrochemically active sites within the electrode material. Defect engineering enhances these properties by introducing oxygen vacancies and dopant atoms that increase charge storage capacity and improve electron transport. Defect-rich metal oxides such as MnO_2 , RuO_2 , NiO , and Co_3O_4 exhibit enhanced pseudocapacitive behavior due to increased redox activity and improved electrolyte accessibility. Oxygen vacancies facilitate ion diffusion within the electrode structure, while dopants modify the electronic conductivity and structural stability. As a result, defect-engineered supercapacitor electrodes often display higher specific capacitance, improved energy density, and superior long-term cycling performance. These characteristics make defect engineering an essential strategy for advancing high-performance energy storage systems (see **Fig. 26**).

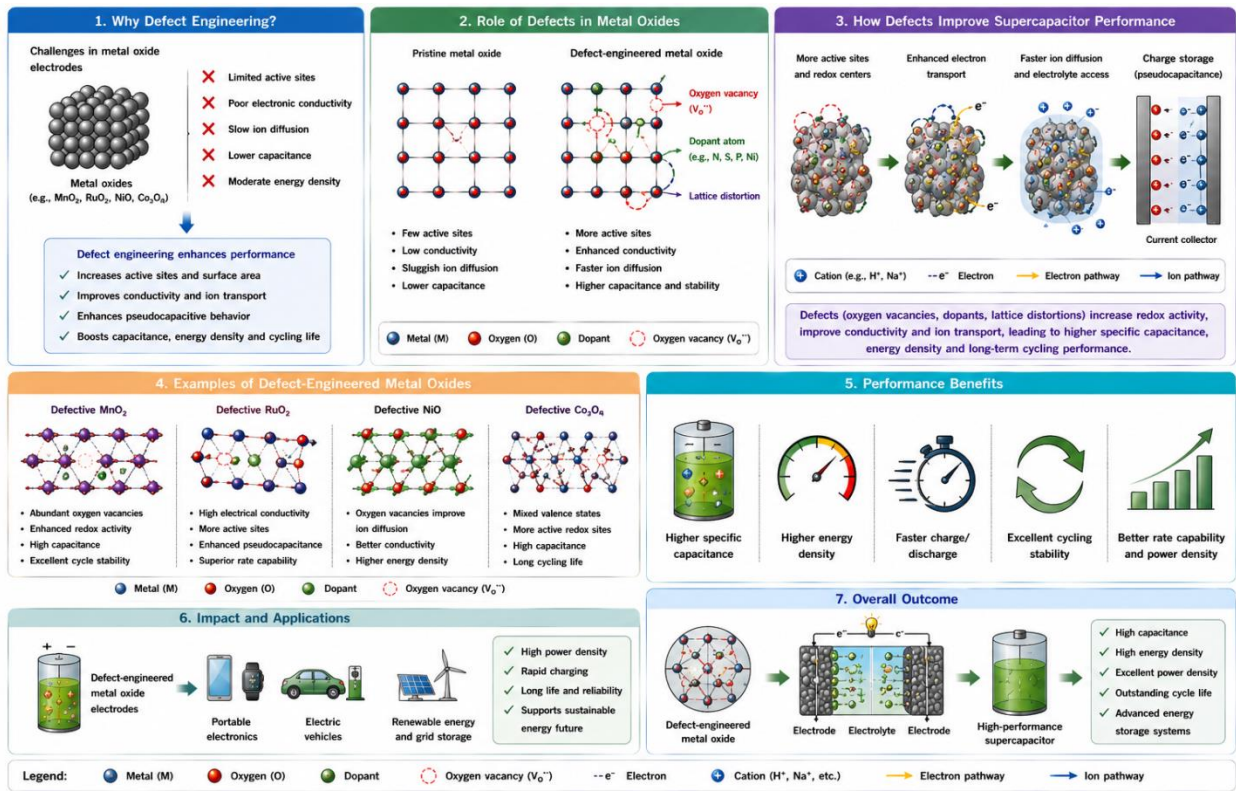


Fig. 26. Defect-engineered metal oxide electrodes for supercapacitors, showing enhanced active sites, electrical conductivity, ion diffusion, pseudocapacitance, energy density, and cycling stability.

SODIUM-ION BATTERIES

Sodium-ion batteries have emerged as a promising alternative to lithium-ion batteries because sodium is abundant, inexpensive, and widely distributed throughout the Earth's crust. However, the larger ionic radius of sodium ions presents challenges related to ion diffusion and structural stability. Defect engineering offers an effective solution by creating expanded diffusion pathways and reducing migration barriers within electrode materials. The introduction of oxygen vacancies and dopants enhances sodium-ion mobility and improves electronic conductivity. Defect-rich TiO₂, V₂O₅, Fe₂O₃, and MnO₂ electrodes have demonstrated improved sodium storage capacity and rate performance. Furthermore, engineered defects help accommodate the volume changes associated with sodium insertion and extraction, thereby enhancing cycling stability. These advantages position defect-engineered metal oxides as key materials for the future development of cost-effective and sustainable sodium-ion battery technologies (see Fig. 27).

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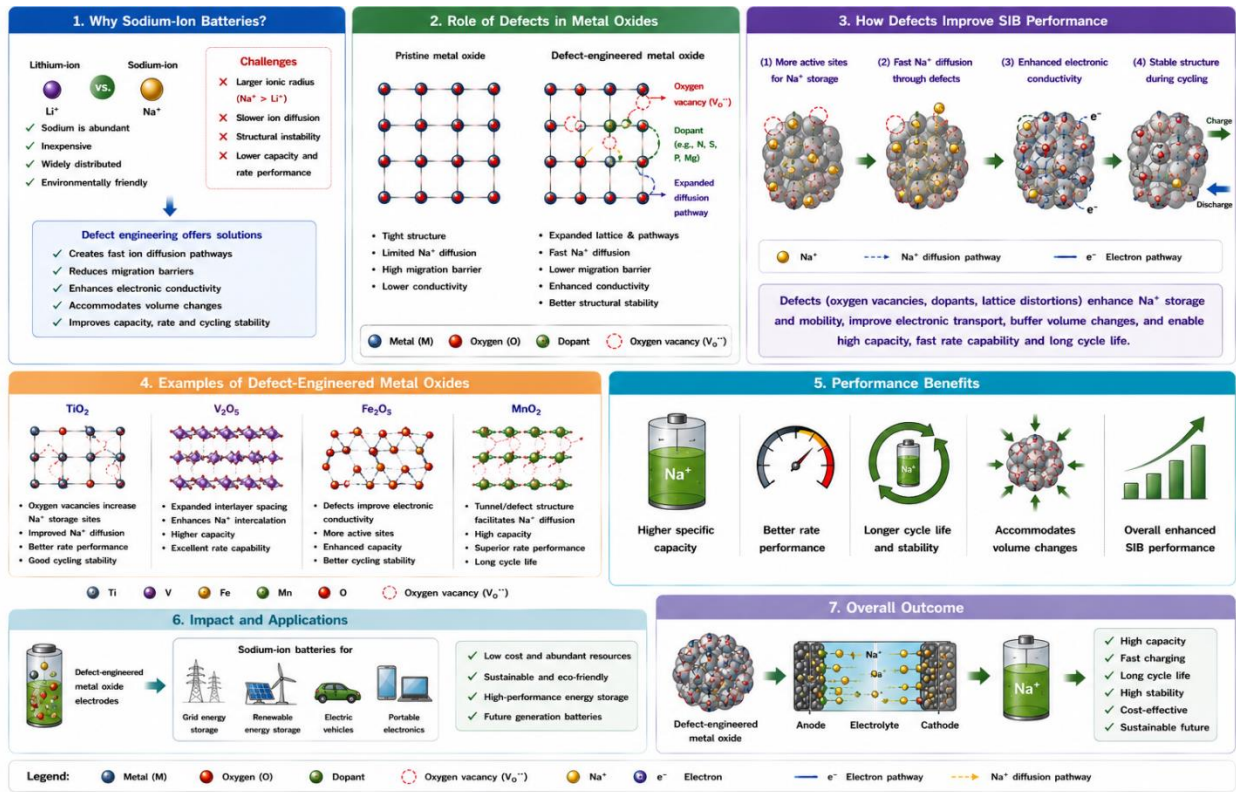


Fig. 27. Defect-engineered metal oxide electrodes for sodium-ion batteries, showing enhanced sodium-ion diffusion, electronic conductivity, storage capacity, rate performance, and cycling stability.

GAS SENSORS

Gas sensing is another important application of defect-engineered metal oxides. Gas sensors based on semiconducting oxides operate through changes in electrical resistance caused by interactions between gas molecules and the sensor surface. The sensitivity and selectivity of these sensors depend largely on the number of available adsorption sites and the efficiency of charge transfer processes. Defect engineering enhances sensor performance by increasing surface reactivity and promoting electron exchange between adsorbed gases and the sensing material (see **Fig. 28**).

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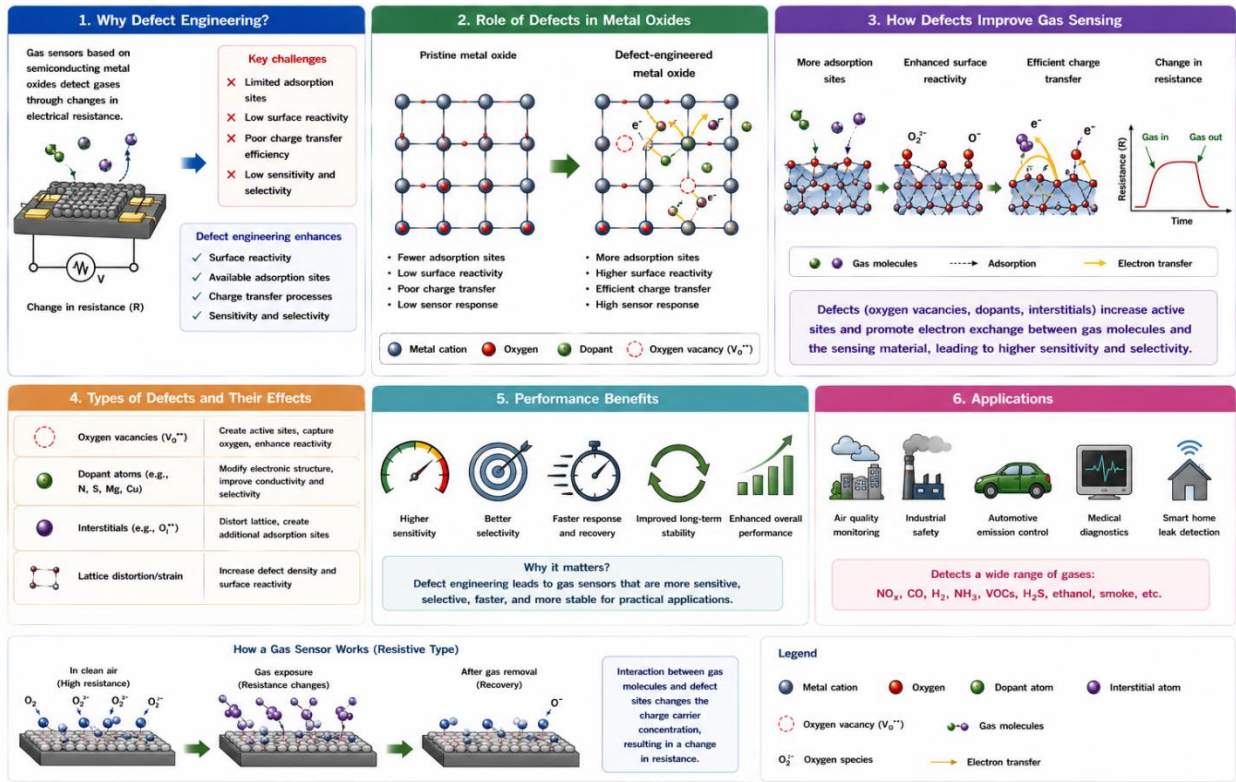


Fig. 28. Defect-engineered metal oxide gas sensors, showing enhanced gas adsorption, charge transfer, resistance change, sensitivity, selectivity, and response–recovery performance.

NO₂ SENSING

Nitrogen dioxide is a highly toxic air pollutant that poses significant environmental and health risks. Accurate detection of NO₂ at low concentrations is therefore essential for environmental monitoring and industrial safety. Oxygen vacancies serve as highly active adsorption sites for NO₂ molecules, increasing the interaction between the gas and the sensor surface. This enhanced adsorption results in larger changes in electrical resistance and improved detection sensitivity. Defect-engineered ZnO, SnO₂, and WO₃ sensors have demonstrated lower detection limits, faster response times, and improved selectivity toward nitrogen dioxide. The increased density of surface defects facilitates electron transfer processes, making defect engineering a highly effective approach for developing advanced NO₂ sensing technologies (see Fig. 29).

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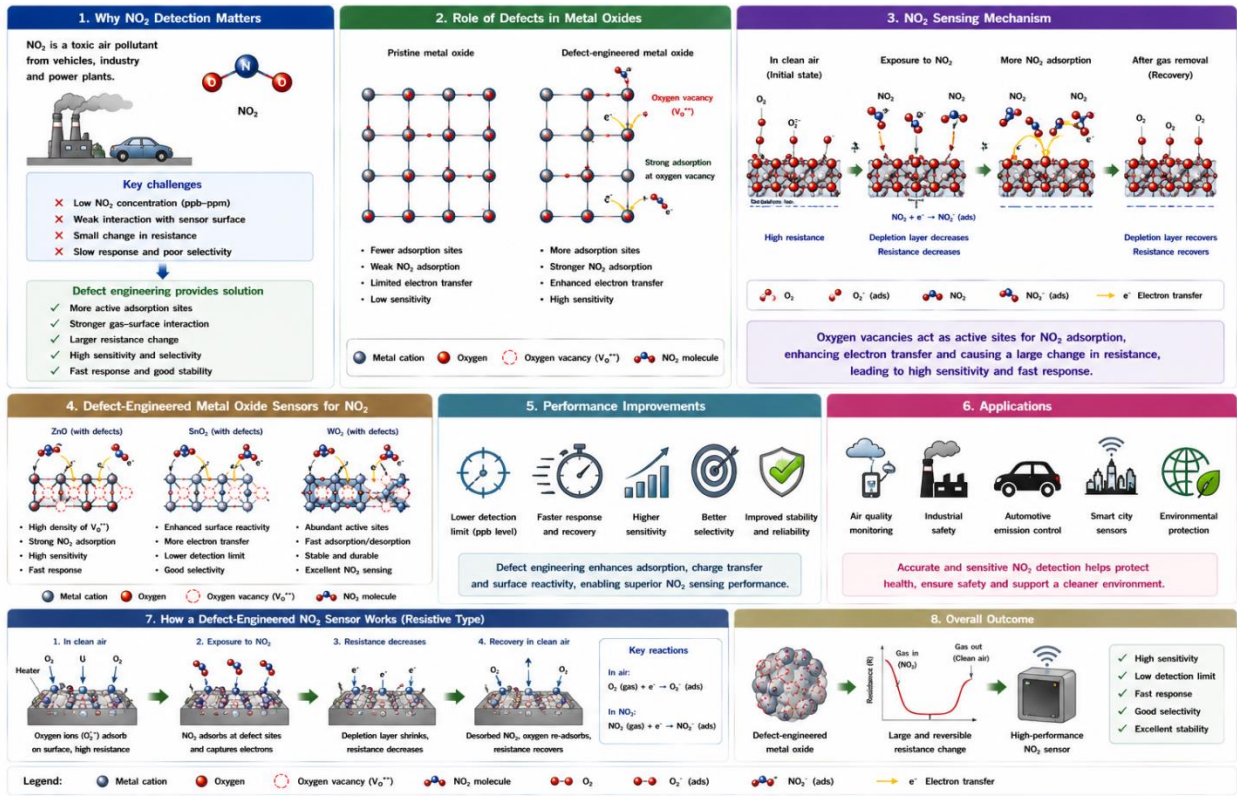


Fig. 29. Defect-engineered metal oxide sensors for NO₂ detection, showing enhanced NO₂ adsorption, electron transfer, resistance response, sensitivity, selectivity, and recovery performance.

H₂ SENSING

Hydrogen is widely used in industrial processes and emerging clean energy systems. However, hydrogen is highly flammable and difficult to detect because it is colorless and odorless. Defect-engineered metal oxides improve hydrogen sensing performance by increasing the number of adsorption sites and enhancing surface reactions between hydrogen molecules and adsorbed oxygen species. Oxygen-deficient ZnO and TiO₂-based sensors exhibit enhanced sensitivity and faster response times due to improved charge transfer mechanisms. In many cases, noble metal catalysts such as palladium or platinum are combined with defect-engineered oxides to further enhance hydrogen adsorption and dissociation. These synergistic effects enable highly efficient hydrogen detection systems for industrial safety and energy applications (see Fig. 30).

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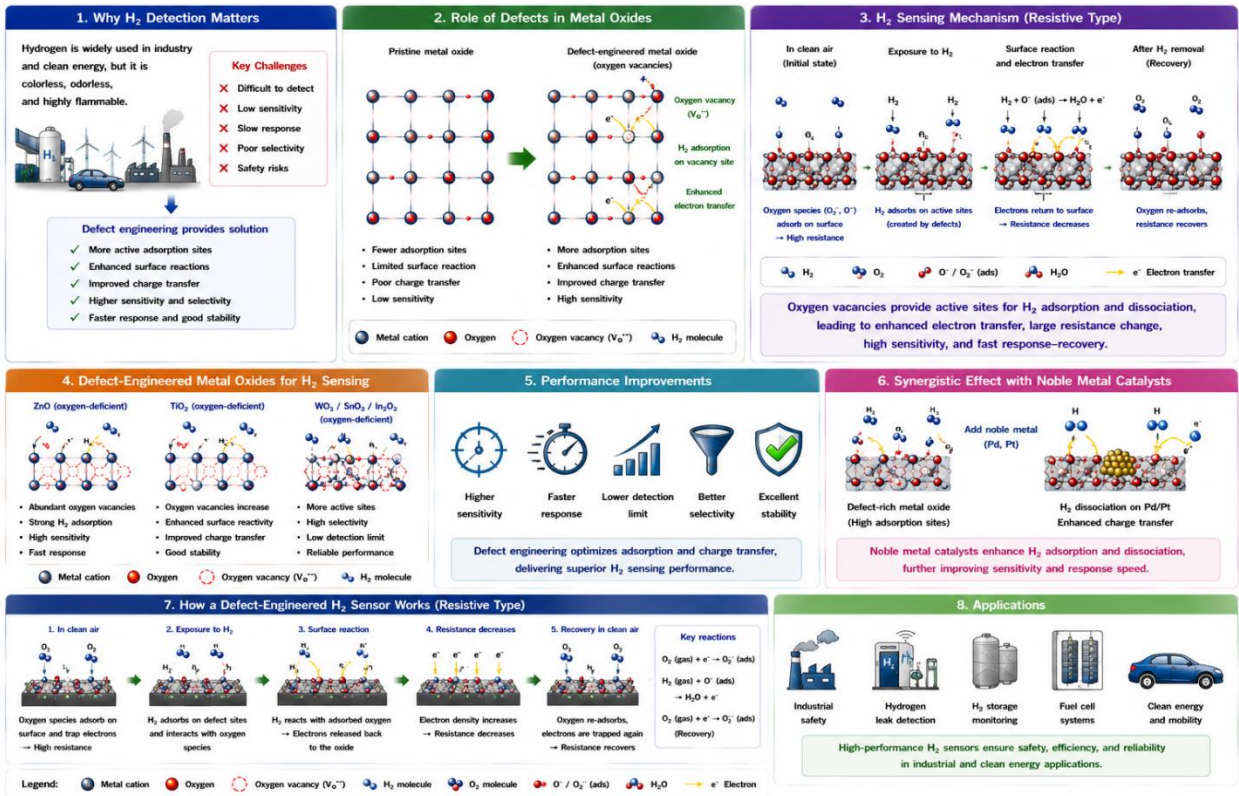


Fig. 30. Defect-engineered metal oxide sensors for hydrogen detection, showing enhanced hydrogen adsorption, surface reactions, charge transfer, sensitivity, response speed, and recovery performance.

VOC DETECTION

Volatile organic compounds (VOCs) such as ethanol, acetone, formaldehyde, benzene, and toluene are common environmental pollutants and health hazards. Defect-engineered metal oxides provide improved VOC detection by increasing adsorption capacity and facilitating oxidation reactions at the sensor surface. Oxygen vacancies play a critical role by enhancing the interaction between VOC molecules and the sensing material. Materials such as ZnO, SnO₂, WO₃, and In₂O₃ with engineered defect structures have demonstrated superior sensitivity, selectivity, and response speed toward various VOCs. These improvements make defect-engineered sensors valuable tools for environmental monitoring, industrial process control, and medical diagnostics such as breath analysis (see **Fig. 31**).

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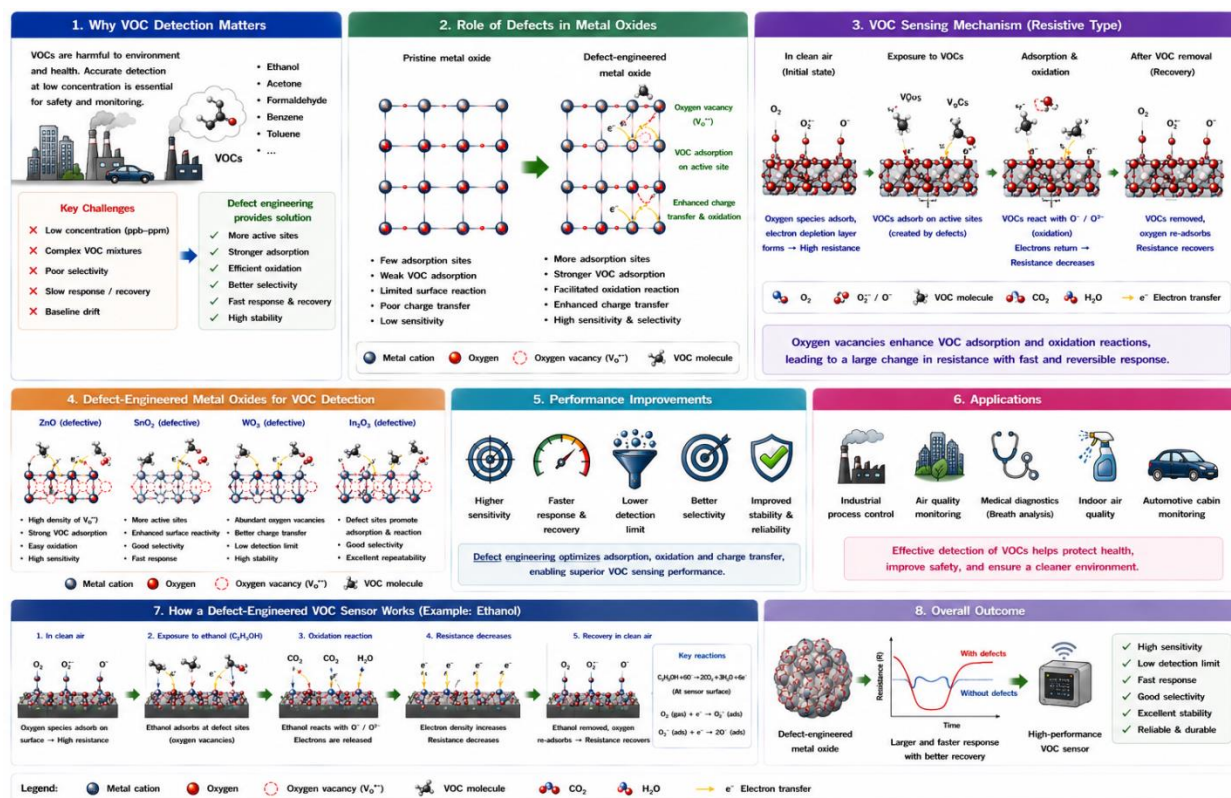


Fig. 31. Defect-engineered metal oxide sensors for VOC detection, showing enhanced VOC adsorption, surface oxidation, charge transfer, sensitivity, selectivity, and response–recovery performance.

ELECTRONIC AND OPTOELECTRONIC DEVICES

Defect engineering has become an indispensable strategy for improving the performance of electronic and optoelectronic devices based on transition metal oxides. The electrical conductivity, carrier concentration, optical transparency, charge transport behavior, and interfacial properties of metal oxides are strongly influenced by the presence of defects. By carefully controlling defect concentration and distribution, researchers can tailor the electronic structure of these materials to meet the requirements of various applications, including solar cells, transparent conducting electrodes, memory devices, photodetectors, and light-emitting systems. Defect engineering enables the optimization of both bulk and surface properties, thereby enhancing device efficiency, stability, and reliability (see **Fig. 32**).

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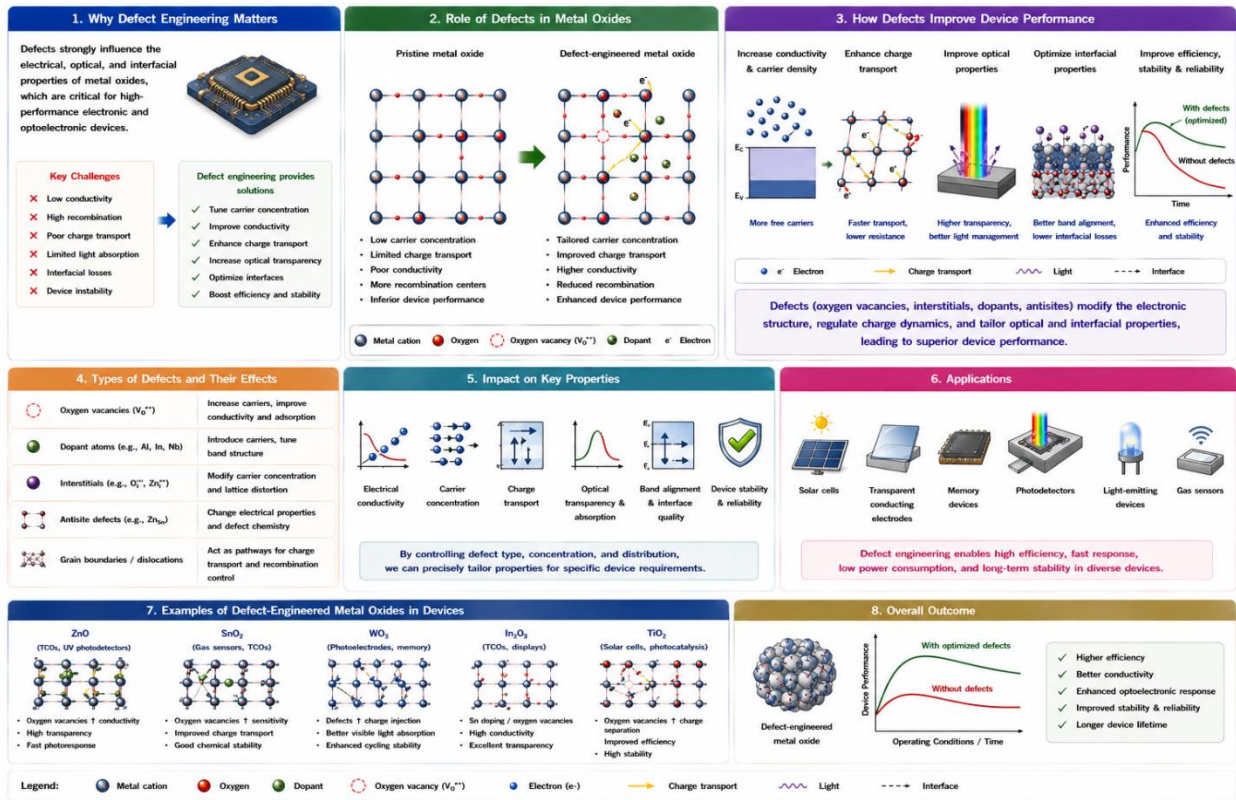


Fig. 32. Defect engineering in metal oxides for electronic and optoelectronic devices, showing improved conductivity, charge transport, optical properties, interfacial performance, efficiency, and stability.

SOLAR CELLS

Solar cells convert sunlight directly into electrical energy through photovoltaic processes. Transition metal oxides such as TiO₂, ZnO, SnO₂, and NiO are widely used as electron transport layers, hole transport layers, and interfacial materials in various photovoltaic technologies, including dye-sensitized solar cells, perovskite solar cells, and organic solar cells. The efficiency of these devices depends heavily on charge generation, separation, transport, and collection processes. Defect engineering significantly improves photovoltaic performance by modifying the band structure and enhancing carrier mobility. Oxygen vacancies can increase electrical conductivity and facilitate charge transport, while controlled doping can optimize energy-level alignment between different device layers. However, excessive defect concentrations may create recombination centers that reduce device efficiency. Therefore, careful optimization of defect density is essential. Numerous studies have demonstrated that defect-engineered TiO₂ and SnO₂ electron transport layers improve charge extraction efficiency, reduce recombination losses, and increase overall power conversion efficiency. As solar energy technologies continue to advance, defect engineering remains a crucial tool for improving device performance and long-term operational stability (see Fig. 33).

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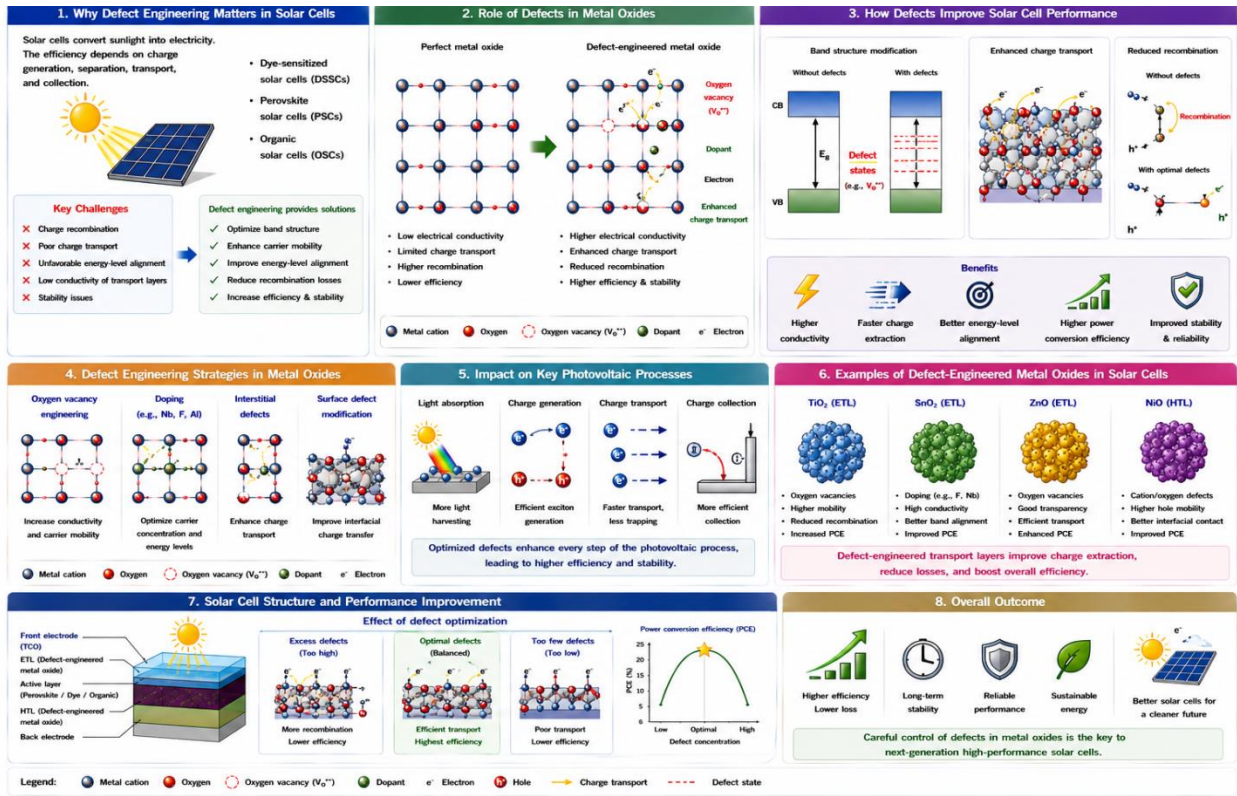


Fig. 33. Defect-engineered metal oxides for solar cells, showing improved light absorption, charge separation, charge transport, reduced recombination, power conversion efficiency, and device stability.

TRANSPARENT CONDUCTORS

Transparent conducting oxides (TCOs) are essential components in modern optoelectronic devices because they combine high optical transparency with excellent electrical conductivity. Common TCO materials include ZnO, SnO₂, In₂O₃, and their doped derivatives. These materials are widely used in displays, touchscreens, photovoltaic modules, smart windows, and light-emitting diodes. Defect engineering plays a central role in controlling the carrier concentration of transparent conductors. Oxygen vacancies often act as donor defects, providing free electrons that enhance conductivity. Similarly, doping with elements such as aluminum, gallium, fluorine, and indium can significantly increase carrier density while maintaining optical transparency. The challenge lies in balancing conductivity and transparency because excessive defect concentrations may increase optical scattering and absorption. Through precise defect control, researchers have developed highly conductive transparent oxides that meet the demanding requirements of next-generation optoelectronic devices (see Fig. 34).

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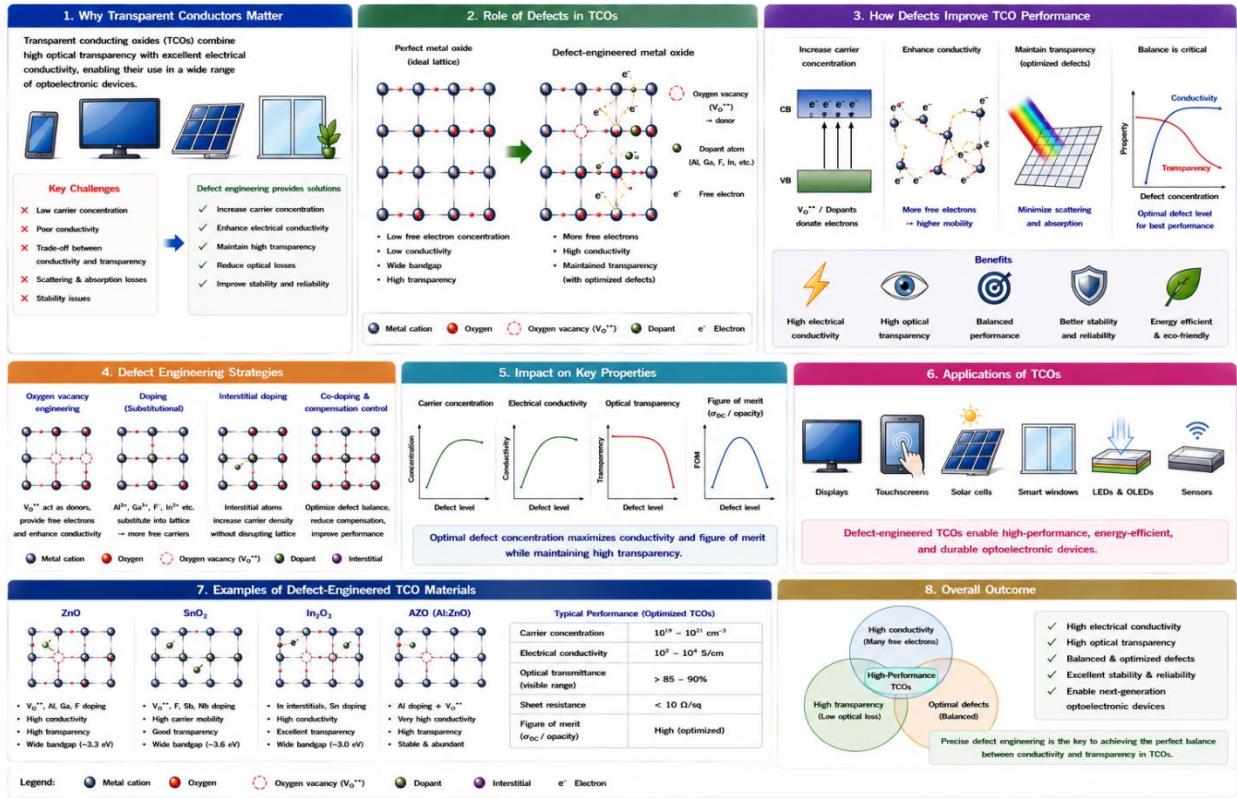


Fig. 34. Defect-engineered transparent conducting oxides, showing the balance between electrical conductivity and optical transparency for advanced optoelectronic applications.

MEMORY DEVICES

The increasing demand for high-density and energy-efficient data storage systems has stimulated extensive research into oxide-based memory devices. Among these technologies, resistive random-access memory (ReRAM) has attracted particular attention due to its simple structure, fast switching speed, low power consumption, and non-volatile data storage capability. The operation of many oxide-based memory devices relies directly on defect dynamics, especially the migration and redistribution of oxygen vacancies. In resistive switching materials such as TiO_2 , HfO_2 , ZnO , and CeO_2 , oxygen vacancies form conductive filaments that can be created or disrupted by an applied electric field. This process allows the material to switch between high-resistance and low-resistance states, representing binary information. Defect engineering enables precise control over filament formation, switching voltage, endurance, and retention characteristics. Consequently, defect-engineered metal oxides have become key materials for emerging memory technologies and neuromorphic computing systems designed to mimic biological neural networks (see Fig. 35).

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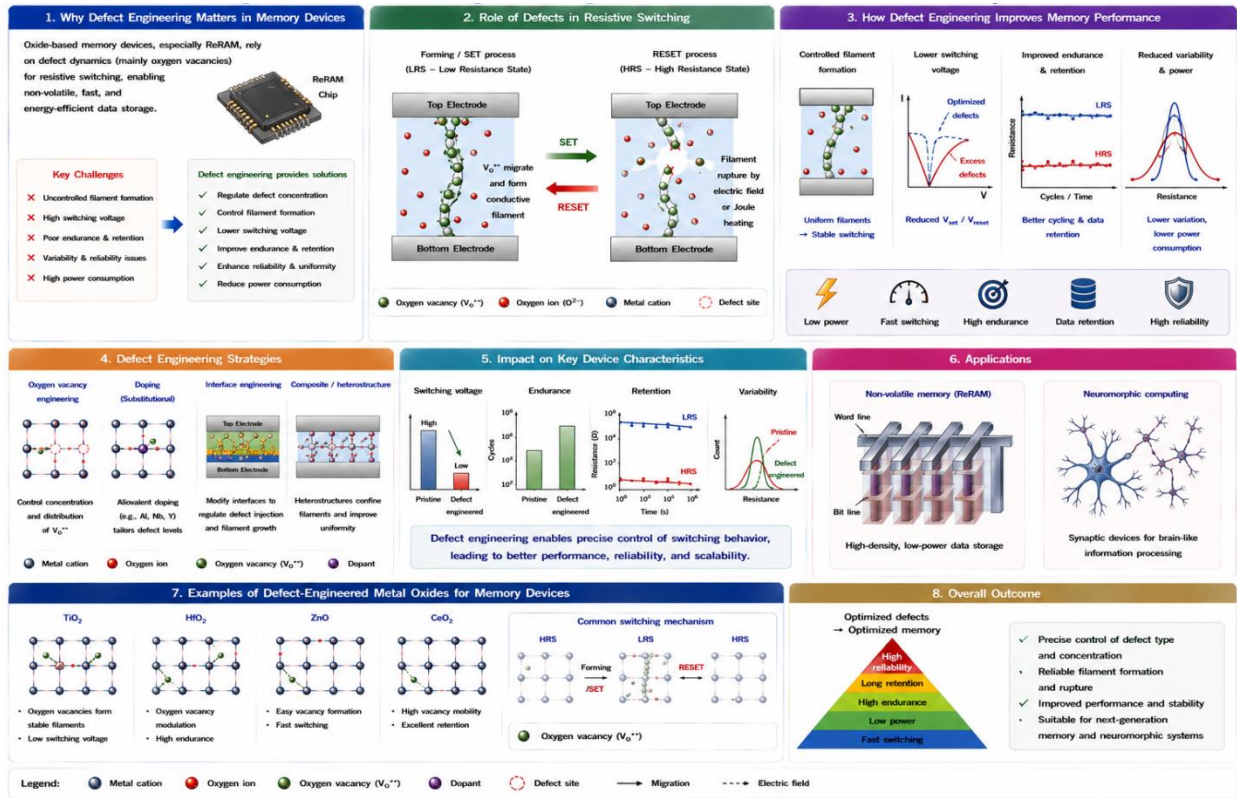


Fig. 35. Defect-engineered metal oxide memory devices, showing oxygen-vacancy migration, conductive filament formation and rupture, resistive switching, and improved memory performance.

BIOMEDICAL APPLICATIONS

The unique physicochemical properties of defect-engineered metal oxides have generated increasing interest in biomedical applications. Controlled defect structures can significantly influence surface chemistry, biological interactions, reactive oxygen species generation, and drug adsorption behavior. These characteristics have enabled the development of advanced materials for antibacterial treatments, targeted drug delivery systems, and highly sensitive biosensors. The ability to tailor defect concentrations provides opportunities for optimizing both therapeutic effectiveness and biocompatibility (see Fig. 36).

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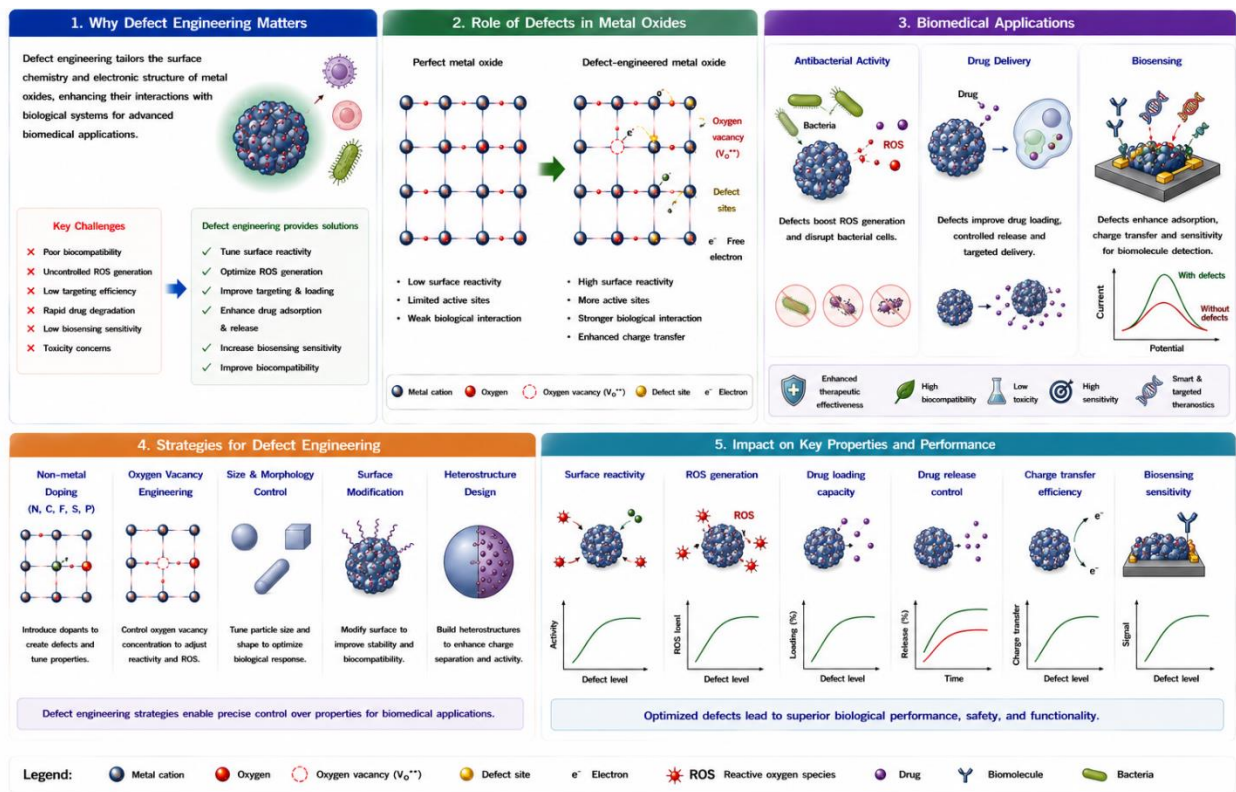


Fig. 36. Biomedical applications of defect-engineered metal oxides, showing enhanced antibacterial activity, drug delivery, biosensing, reactive oxygen species generation, and biocompatibility.

ANTIBACTERIAL ACTIVITY

Bacterial infections remain a major challenge in healthcare, particularly due to the growing prevalence of antibiotic-resistant microorganisms. Defect-engineered metal oxide nanoparticles have emerged as promising antibacterial agents because of their ability to generate reactive oxygen species (ROS) and disrupt bacterial cellular functions. Oxygen vacancies and surface defects play a crucial role in enhancing antibacterial activity by increasing the production of reactive species such as hydroxyl radicals, superoxide radicals, and hydrogen peroxide. These reactive species damage bacterial cell membranes, proteins, enzymes, and genetic material, ultimately leading to cell death. Defect-rich ZnO, TiO₂, CeO₂, and CuO nanoparticles have demonstrated strong antibacterial activity against both Gram-positive and Gram-negative bacteria. Additionally, defect engineering can improve nanoparticle interaction with bacterial surfaces by increasing surface charge and adsorption capability. These properties make defect-engineered metal oxides attractive candidates for antimicrobial coatings, wound dressings, medical implants, and water disinfection systems (see Fig. 37).

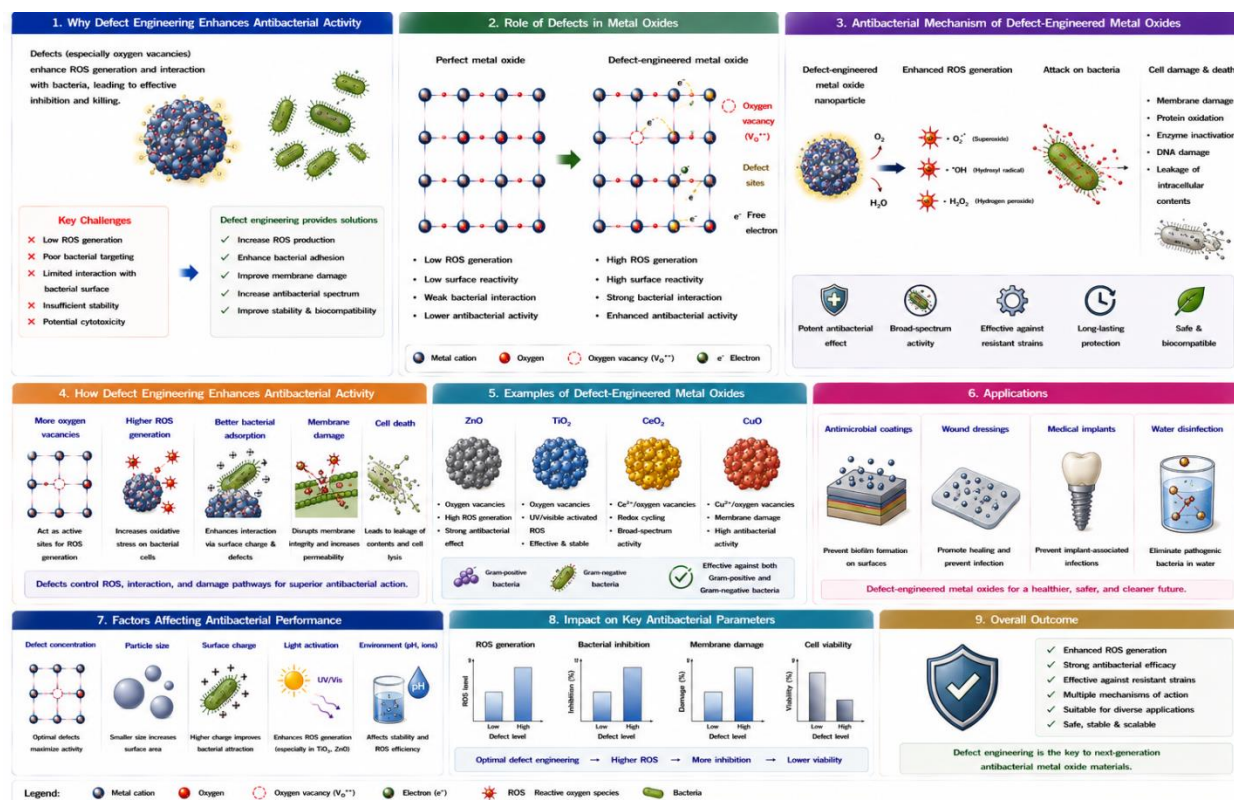


Fig. 37. Antibacterial activity of defect-engineered metal oxides through enhanced reactive oxygen species generation and bacterial cell damage.

DRUG DELIVERY

Targeted drug delivery systems aim to transport therapeutic agents directly to diseased tissues while minimizing side effects and improving treatment efficiency. Defect-engineered metal oxides offer several advantages for drug delivery applications, including large surface area, tunable porosity, controlled surface chemistry, and enhanced adsorption capacity. Structural defects and oxygen vacancies create additional active sites that facilitate drug loading and retention. The release behavior of therapeutic agents can be regulated through defect concentration, surface functionalization, and environmental stimuli such as pH, temperature, and light exposure. For example, mesoporous defect-engineered TiO_2 and CeO_2 nanoparticles have been investigated as carriers for anticancer drugs, antibiotics, and anti-inflammatory agents. Their ability to combine drug delivery with imaging, phototherapy, or antioxidant activity further enhances their potential in multifunctional biomedical platforms. Continued advances in defect engineering are expected to improve the precision and effectiveness of future nanomedicine technologies (see **Fig. 38**).

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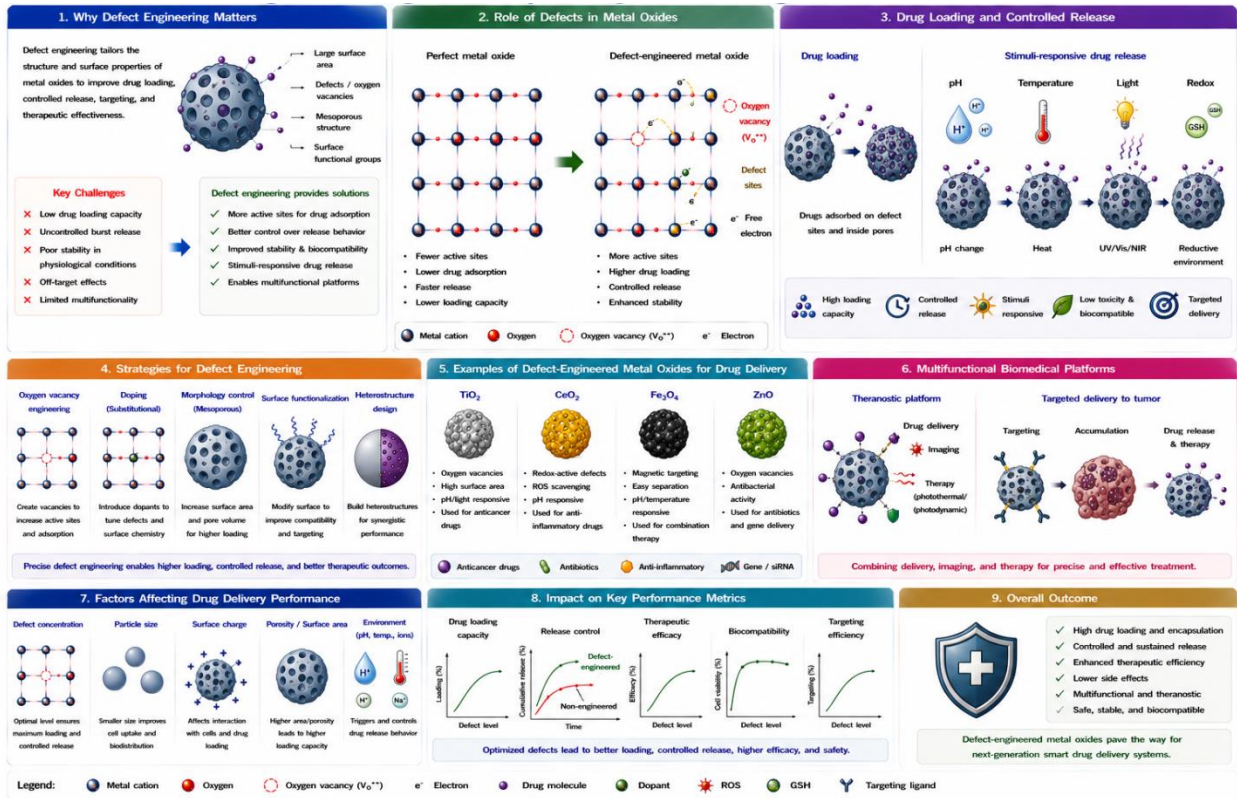


Fig. 38. Drug delivery using defect-engineered metal oxides, showing enhanced drug loading, controlled release, targeted delivery, and improved therapeutic performance.

BIOSENSORS

Biosensors are analytical devices that convert biological interactions into measurable electrical, optical, or electrochemical signals. The sensitivity and selectivity of biosensors depend strongly on the properties of the sensing material, particularly its surface area, conductivity, and electron transfer capability. Defect engineering significantly enhances these properties by increasing the number of active sites and facilitating charge transport. Oxygen vacancies and dopant-induced defects improve the adsorption of biomolecules and accelerate electron transfer between biological recognition elements and electrode surfaces. Defect-engineered metal oxides such as ZnO, TiO₂, CeO₂, and SnO₂ have been widely used in biosensors for the detection of glucose, cholesterol, proteins, nucleic acids, cancer biomarkers, and pathogenic microorganisms. These materials often exhibit lower detection limits, faster response times, and improved signal stability compared with conventional sensing materials. As healthcare increasingly moves toward personalized medicine and point-of-care diagnostics, defect-engineered biosensors are expected to play an increasingly important role in disease diagnosis and monitoring (see **Fig. 39**).

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Fig. 39. Defect-engineered metal oxide biosensors, showing enhanced biomolecule adsorption, electron transfer, sensitivity, selectivity, and signal stability for disease diagnosis and monitoring.

COMPARATIVE PERFORMANCE ANALYSIS

The remarkable progress achieved through defect engineering has led to extensive investigations comparing different transition metal oxides, defect types, and defect concentrations. Comparative performance analysis is essential for identifying the most effective materials and optimization strategies for specific applications. The performance of defect-engineered metal oxides depends not only on the type of defect introduced but also on defect density, defect distribution, synthesis method, crystal structure, and operating environment. Understanding these relationships is critical for designing materials with superior functionality and long-term stability.

COMPARISON OF DIFFERENT METAL OXIDES

Different transition metal oxides respond differently to defect engineering because of variations in their crystal structures, electronic configurations, and defect formation energies. Titanium dioxide (TiO₂) remains one of the most extensively studied materials due to its excellent chemical stability, low cost, and strong photocatalytic activity. Oxygen vacancy engineering in TiO₂ significantly enhances visible-light absorption and charge separation, making it highly effective for photocatalytic and photovoltaic applications. However, its relatively wide bandgap still limits solar energy utilization under certain conditions. Zinc oxide (ZnO) is another widely investigated material because of its high electron mobility and strong sensitivity to surface defects. Defect-engineered ZnO performs exceptionally well in gas sensing and photocatalytic applications, although it may suffer from photocorrosion and stability issues in harsh environments. Cerium oxide (CeO₂) possesses unique redox properties associated with the reversible transition between Ce³⁺ and Ce⁴⁺ states. This characteristic makes defect-engineered CeO₂ particularly attractive for catalytic and environmental applications. Tungsten oxide (WO₃) exhibits strong visible-light absorption and excellent gas sensing capabilities, while tin oxide (SnO₂) remains one of the most important materials for chemical sensing and transparent conductive applications. Each material offers distinct advantages and limitations, highlighting the importance of selecting appropriate defect engineering strategies according to the target application (see Fig. 40).

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Metal Oxide	TiO ₂ (Titanium Dioxide)	ZnO (Zinc Oxide)	CeO ₂ (Cerium Oxide)	WO ₃ (Tungsten Oxide)	SnO ₂ (Tin Oxide)
Crystal Structure	Anatase / Rutile	Wurtzite	Fluorite	Monoclinic	Rutile
Key Defect Engineered	Oxygen vacancies (V _O ^{••}) Ti ³⁺ centers, Doping (N, C, S)	Oxygen vacancies (V _O ^{••}) Zn interstitials, Doping (Al, Ga)	Oxygen vacancies (V _O ^{••}) Ce ³⁺ /Ce ⁴⁺ redox couple	Oxygen vacancies (V _O ^{••}) W ⁵⁺ /W ⁶⁺ , Non-stoichiometry	Oxygen vacancies (V _O ^{••}) Sn interstitials, Doping (F, Sb)
Electronic Properties	- Wide bandgap ~3.0–3.2 eV - Defects narrow bandgap - Improved charge separation	- Wide bandgap ~3.2–3.4 eV - High electron mobility - Defects create shallow levels	- Bandgap ~2.9–3.2 eV - Ce³⁺/Ce⁴⁺ redox enhances oxygen storage & mobility	- Bandgap ~2.6–2.8 eV - Strong visible-light absorption - Defects improve conductivity	- Wide bandgap ~3.6 eV - High conductivity - Defects boost electron density
Key Advantages	- Excellent chemical stability - Strong photocatalytic activity - Abundant and non-toxic - Good for energy & environmental applications	- High electron mobility - High sensitivity to defects - Excellent gas sensing - Strong UV photocatalysis	- Unique Ce³⁺/Ce⁴⁺ redox - Oxygen storage capacity - Excellent catalytic activity - Good environmental catalyst	- Strong visible-light absorption - High gas sensing performance - Good electrochromic behavior - Tunable conductivity	- High transparency & conductivity - Excellent chemical stability - Superior gas sensing - Widely used in electronics
Limitations	- Wide bandgap limits visible light utilization - Recombination of charge carriers	- Photocorrosion in harsh environments - Lower stability in acidic conditions	- Lower conductivity than ZnO/SnO₂ - Sintering at high temperature - More expensive than TiO₂ or ZnO	- Poor stability in humidity - Slow response recovery - Moderate conductivity	- Lower catalytic activity compared to CeO₂ - Sensitivity affected by humidity
Major Applications	Photocatalysis, Solar cells, Water treatment	Gas sensors, UV photocatalysis, Antibacterial coatings	Catalysis, Environmental remediation, Energy storage	Gas sensors, Electrochromic devices, Photocatalysis	Gas sensors, Transparent conductors, Electronics
Overall Comparison	Each metal oxide exhibits unique properties and responds differently to defect engineering. Selecting the right oxide and defect strategy is crucial for maximizing performance in specific applications.				Metal cation Oxygen Oxygen vacancy (V_O^{••}) Defect energy level

Fig. 40. Comparison of different metal oxides under defect engineering

EFFECT OF DEFECT DENSITY

The concentration of defects within a metal oxide plays a decisive role in determining its overall performance. At low defect densities, the number of active sites and charge carriers may be insufficient to produce significant performance improvements. As defect concentration increases, beneficial effects such as enhanced conductivity, improved catalytic activity, greater adsorption capacity, and faster ion diffusion become more pronounced. However, excessive defect densities can have detrimental consequences. High concentrations of vacancies or dopants may introduce structural instability, increase carrier recombination rates, and reduce crystallinity. In photocatalytic systems, excessive defects may act as recombination centers that decrease quantum efficiency. Similarly, in energy storage devices, excessive defect accumulation can lead to capacity fading and mechanical degradation during cycling. Therefore, an optimal defect density typically exists where the positive effects of defect engineering are maximized while negative effects remain minimal. Determining this optimum remains a major focus of current research and is often highly dependent on the specific material and application.

ADVANTAGES AND LIMITATIONS

Defect engineering offers numerous advantages that have significantly expanded the functionality and application range of transition metal oxides. One of the most important benefits is the ability to tailor the electronic structure of materials without fundamentally altering their crystal framework. Through the introduction of oxygen vacancies, dopants, lattice distortions, and interface defects, researchers can effectively regulate bandgap energy, carrier concentration, conductivity, and catalytic activity. This flexibility allows a single material to be optimized for different applications, ranging from photocatalysis and energy storage to sensing and biomedical technologies. Another major advantage of defect engineering is the enhancement of surface activity. Defects create additional active sites that promote adsorption, charge transfer, and chemical reactions. In photocatalytic systems, defects improve light absorption and suppress electron-hole recombination, leading to higher quantum efficiencies. In battery electrodes, defects facilitate ion diffusion and increase storage capacity. In gas sensors, they enhance sensitivity and response speed by providing more adsorption centers for target gas molecules. Furthermore, defect engineering can improve

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material selectivity, reduce operating temperatures, and enable multifunctional performance that combines several desirable properties within a single material system. Despite these advantages, defect engineering also faces several important limitations. Precise control of defect concentration and distribution remains challenging because defect formation often depends sensitively on synthesis conditions such as temperature, atmosphere, precursor composition, and processing time. Small variations in fabrication parameters may produce significant differences in material properties and performance. Additionally, many defects are thermodynamically unstable and may gradually disappear during operation, leading to performance degradation over time.

Another limitation is that excessive defect concentrations can negatively affect material properties. High defect densities may increase charge carrier recombination, reduce crystallinity, weaken mechanical stability, and accelerate structural degradation. The characterization of defects also presents considerable challenges because many defect structures exist at the atomic scale and require sophisticated analytical techniques such as electron paramagnetic resonance spectroscopy, positron annihilation spectroscopy, synchrotron X-ray methods, and advanced transmission electron microscopy. Consequently, achieving reliable and reproducible defect control remains one of the major challenges in practical applications of defect-engineered materials.

CHALLENGES AND FUTURE PERSPECTIVES

Although defect engineering has demonstrated tremendous potential for improving the performance of transition metal oxides, several scientific and technological challenges must be overcome before widespread commercial implementation can be achieved. Current research efforts are increasingly focused on understanding defect formation mechanisms, improving defect stability, developing scalable synthesis methods, and integrating computational approaches for rational materials design. Addressing these challenges will be essential for translating laboratory-scale successes into practical technologies capable of meeting future energy, environmental, and healthcare demands.

STABILITY ISSUES

One of the most significant challenges facing defect-engineered metal oxides is long-term stability. Many beneficial defects, particularly oxygen vacancies, exist in metastable states and tend to disappear over time as the material approaches thermodynamic equilibrium. Environmental factors such as temperature, humidity, oxygen exposure, electrical bias, and repeated operational cycling can accelerate defect annihilation and structural relaxation processes. The loss of defects often leads to deterioration in material performance. In photocatalysts, vacancy annihilation may reduce visible-light absorption and catalytic activity. In batteries and supercapacitors, structural degradation associated with defect evolution can cause capacity fading and reduced cycle life. Similarly, gas sensor sensitivity may decline as active defect sites become passivated. To address these challenges, researchers are exploring approaches such as defect stabilization through co-doping, interface engineering, heterostructure formation, and protective surface coatings. The development of stable defect architectures remains a critical requirement for practical applications.

SCALABILITY AND INDUSTRIAL PRODUCTION

Most defect-engineered metal oxides are currently synthesized under carefully controlled laboratory conditions that may not be suitable for large-scale manufacturing. Techniques such as plasma treatment, vacuum annealing, laser processing, and atomic-layer deposition often require specialized equipment and significant energy input, increasing production costs. Furthermore, maintaining consistent defect concentrations across large material volumes remains technically challenging. Industrial applications require synthesis methods that are cost-effective, reproducible, environmentally friendly, and compatible with high-throughput production. Researchers are therefore investigating scalable approaches such as chemical vapor deposition, spray pyrolysis, hydrothermal synthesis, sol-gel processing, and continuous-flow manufacturing systems. Achieving precise defect control while maintaining economic viability will be essential for the

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commercialization of defect-engineered materials in energy storage devices, environmental technologies, and electronic systems.

TOXICITY AND ENVIRONMENTAL CONCERNS

As the production and use of nanostructured metal oxides continue to increase, concerns regarding their environmental and biological safety have become increasingly important. Defect engineering may alter the chemical reactivity, dissolution behavior, and biological interactions of nanoparticles, potentially affecting their toxicity profiles. While enhanced reactivity is beneficial for catalytic applications, it may also increase the generation of reactive oxygen species that can cause unintended biological damage. The release of defect-engineered nanoparticles into air, water, and soil environments raises concerns regarding bioaccumulation, ecological toxicity, and long-term environmental persistence. Comprehensive toxicological studies are therefore necessary to evaluate the safety of these materials throughout their life cycle. Future research should focus on developing environmentally benign synthesis methods, biodegradable materials, and effective recycling strategies. Regulatory frameworks will also be needed to ensure the safe use of defect-engineered nanomaterials in commercial applications (see Fig. 41).

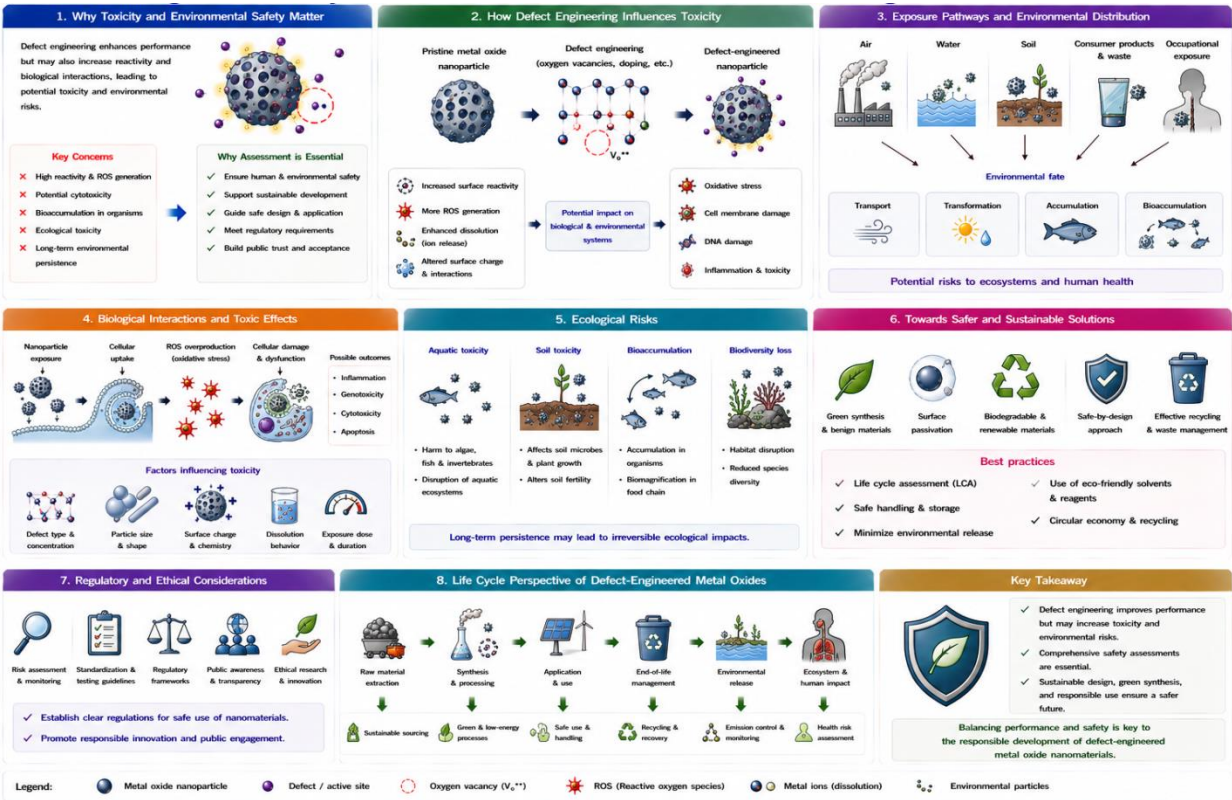


Fig. 41. Toxicity and environmental concerns of defect-engineered metal oxides

AI AND MACHINE LEARNING IN MATERIALS DESIGN

Artificial intelligence (AI) and machine learning (ML) are emerging as transformative tools for accelerating the discovery and optimization of defect-engineered materials. Traditional experimental approaches often require extensive trial-and-error procedures that consume considerable time and resources. AI-driven methods can analyze large datasets, identify hidden relationships between material composition and performance, and predict optimal defect configurations with unprecedented speed. Machine learning algorithms can be trained using experimental and computational databases to predict defect formation energies, electronic properties, catalytic activity, and stability. Combined with density functional theory calculations and high-throughput screening methods, AI enables rapid exploration of vast compositional spaces that would be impossible to investigate experimentally. Furthermore, autonomous laboratories integrating robotics, real-time characterization, and machine learning are beginning to demonstrate the

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ability to perform self-directed materials discovery. These advances are expected to significantly accelerate the development of next-generation defect-engineered metal oxides (see Fig. 42).

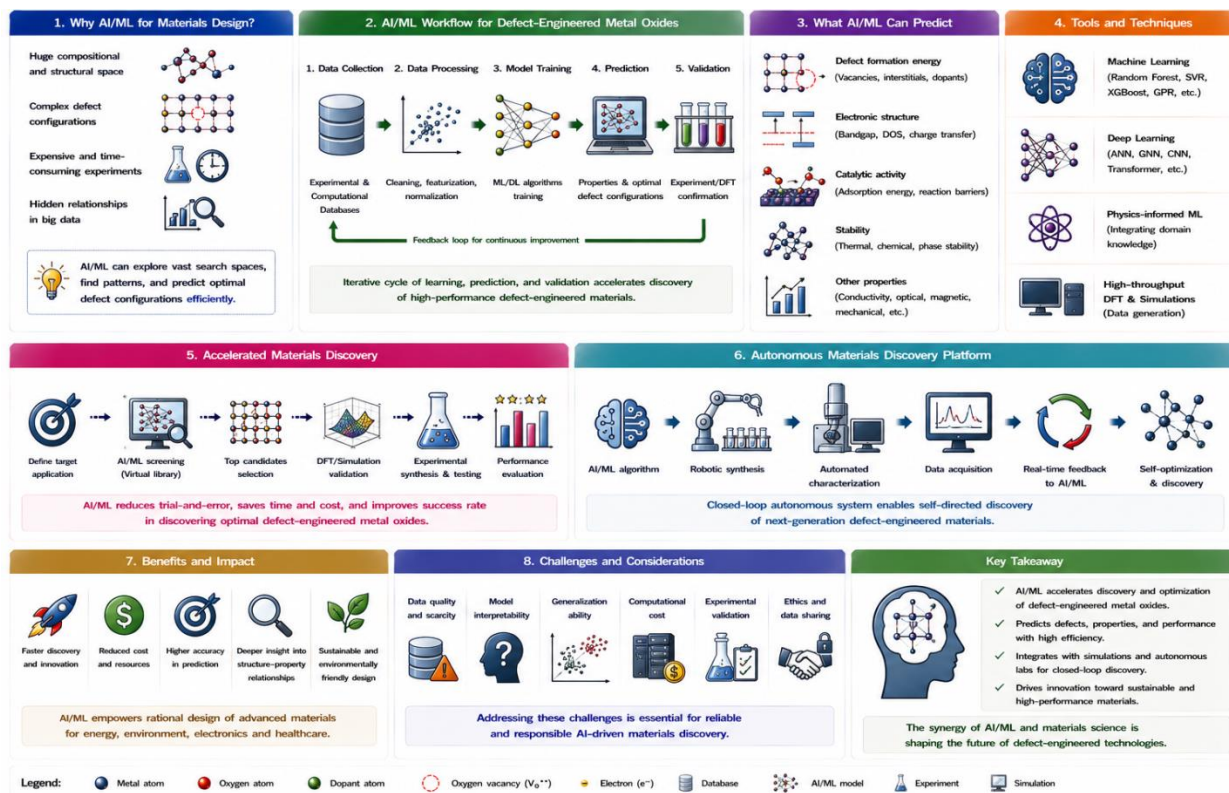


Fig. 42. AI and machine learning in materials design of defect-engineered metal oxides

FUTURE RESEARCH DIRECTIONS

Future research in defect engineering is expected to move beyond the simple introduction of isolated defects toward the development of highly controlled and multifunctional defect architectures. One promising direction involves the simultaneous engineering of multiple defect types, such as combining oxygen vacancies, dopants, and heterointerfaces to achieve synergistic performance enhancements. Understanding the interactions among different defects will be essential for maximizing material functionality. Advanced characterization techniques capable of directly observing defects under operating conditions will also become increasingly important. In situ and operando methods, including synchrotron-based spectroscopy, environmental transmission electron microscopy, and scanning probe techniques, will provide valuable insights into defect evolution during real-time operation. Such information will help establish fundamental relationships between defect structures and material performance. Another important research direction involves integrating defect engineering with emerging technologies such as quantum materials, flexible electronics, wearable sensors, and renewable energy systems. The development of sustainable synthesis methods that minimize environmental impact while maintaining precise defect control will also receive considerable attention. Additionally, AI-assisted materials design is expected to transform the field by enabling predictive defect engineering and accelerating the discovery of high-performance materials.

Ultimately, future progress will depend on interdisciplinary collaboration among materials scientists, chemists, physicists, engineers, computational researchers, and industrial partners. Such collaborative efforts will be crucial for overcoming current limitations and unlocking the full potential of defect-engineered transition metal oxides.

CONCLUSION

Defect engineering has emerged as one of the most powerful strategies for tailoring the properties of transition metal oxides and enhancing their performance across a broad spectrum of technological

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applications. Through the deliberate introduction and manipulation of oxygen vacancies, dopants, surface defects, heterointerfaces, and lattice strain, researchers have gained unprecedented control over the structural, electronic, optical, catalytic, and electrochemical characteristics of these materials. Such modifications enable substantial improvements in charge transport, light absorption, ion diffusion, surface reactivity, and overall functional performance. Among the various defect engineering approaches, oxygen vacancy engineering remains the most extensively investigated because of its profound influence on conductivity, catalytic activity, and adsorption behavior. Elemental doping provides additional opportunities for band structure tuning and defect stabilization, while surface modification, heterostructure formation, and strain engineering offer complementary pathways for enhancing performance. The synergistic combination of these strategies has led to remarkable advances in photocatalysis, hydrogen production, carbon dioxide reduction, pollutant degradation, lithium-ion and sodium-ion batteries, supercapacitors, gas sensors, solar cells, transparent conductors, memory devices, and biomedical technologies. Despite these achievements, several important challenges remain. Long-term defect stability, reproducible defect control, scalable manufacturing processes, and environmental safety considerations continue to limit widespread commercialization. Addressing these issues will require the development of advanced synthesis techniques, real-time characterization methods, and predictive computational tools capable of guiding defect design at the atomic level. Looking forward, the integration of artificial intelligence, machine learning, high-throughput experimentation, and operando characterization techniques is expected to revolutionize the field of defect engineering. These emerging technologies will enable precise control of defect structures, accelerate materials discovery, and facilitate the design of multifunctional materials with unprecedented performance. As global demand for sustainable energy systems, environmental remediation technologies, advanced electronics, and biomedical devices continues to grow, defect-engineered transition metal oxides are expected to play a pivotal role in shaping the next generation of functional materials and enabling a more sustainable technological future.

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