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**Physics of Nanocomposites:
Environmental Applications and Safety Principles**

A Course Manual for Master's Students in Physics

Special Course: Physics of Nanocomposites

Taras Shevchenko National University of Kyiv | 2026

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The textbook "Physics of Nanocomposites: Environmental Applications and Safety Principles" addresses the physical mechanisms underlying the use of nanocomposite materials for solving pressing environmental problems. The book covers nanophysical fundamentals of surface phenomena and size effects, the physics of sorption processes and membrane purification, nanophotocatalysis, physical aspects of nanotoxicology, and principles of sustainable design and life-cycle assessment. The material is presented in a quantitative manner with numerical examples and problem sets, facilitating an interdisciplinary approach to the study of functional nanomaterials.

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APPROVAL

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Preface

This course manual, Physics of Nanocomposites: Environmental Applications and Safety Principles, has been prepared by the academic staff of the Department of Metals Physics, Faculty of Physics, Taras Shevchenko National University of Kyiv. It is intended as a supplementary teaching resource that systematically expands and deepens the material covered in two courses offered by the Department.

For Master's students enrolled in the educational-scientific programme "Physics of Nanosystems," the manual serves as an extended companion to the compulsory course Physics of Nanocomposite Materials (OK-11, 3 ECTS), taught in Semester 2 of the first Master's year. That course provides a broad foundation in the physics, physico-chemical characteristics, and manufacturing principles of nanostructured hetero-phase materials based on metals, ceramics, and polymers. The present manual deepens this foundation by focusing specifically on environmental applications and safety aspects — topics that are rapidly gaining scientific and regulatory importance but are rarely covered in sufficient depth by a single textbook.

For Bachelor's students in the Physics of Nanosystems elective block, the manual complements the fourth-year course Physics of Nanostructured Materials (VK-10), which introduces students to the physics of low-dimensional and nanostructured systems. Chapters 1 and 2 of this manual — covering surface phenomena, quantum size effects, sorption physics, and membrane transport — are directly aligned with topics encountered in that course, allowing advanced undergraduate students to consolidate their knowledge and begin engaging with research-level applications.

A defining feature of this manual is its interdisciplinary character. The subject matter deliberately bridges the boundaries between condensed matter physics, environmental science, materials chemistry, toxicology, and regulatory policy. Chapter 1 establishes the nanophysical foundations — surface-to-volume geometry, quantum confinement, superparamagnetism, and nanosensor physics. Chapter 2 translates these foundations into the language of sorption thermodynamics and membrane transport. Chapter 3 draws on semiconductor physics and photochemistry to explain photocatalytic remediation. Chapter 4 connects nanophysics to nanotoxicology and aerosol biophysics — areas governed as much by medicine and environmental law as by physics. Chapter 5 introduces Life Cycle Assessment and Safe-and-Sustainable-by-Design principles, linking fundamental physical research to materials engineering, environmental regulation, and societal responsibility. This breadth reflects the contemporary reality of nanoscience: no significant advance in nanocomposite technology can be responsibly pursued without addressing its environmental footprint and safety implications throughout the entire material life cycle.

Note on the Use of Artificial Intelligence Tools. *In the preparation of this manual, the authors made use of artificial intelligence (AI) tools in a limited and clearly defined capacity, in full compliance with the Law of Ukraine No. 4742-IX "On Academic Integrity" (signed 29 January 2026, in force from 1 February 2026), which establishes the legal framework for the transparent and responsible use of AI in academic work. Specifically, AI tools were employed for two auxiliary purposes only: (1) Google NotebookLM was used at the early planning stage for brainstorming the structure of chapters and identifying thematic connections between topics; (2) DeepL Write was used for stylistic editing and improving the fluency of the English-language text. All scientific content, physical derivations, numerical examples, pedagogical decisions, and final formulations were developed exclusively by the authors. No AI-generated text has been reproduced verbatim in this manual without independent verification and substantial revision by the authors.*

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Introduction

The escalation of global environmental challenges in the 21st century—including clean water scarcity, climate change, and industrial pollution—has necessitated the development of innovative and sustainable material solutions [1, 2]. Conventional treatment technologies often face limitations such as high energy consumption and the generation of secondary waste. Nanotechnology provides a transformative pathway for environmental engineering, offering high-performance nanocomposite materials [3, 4].

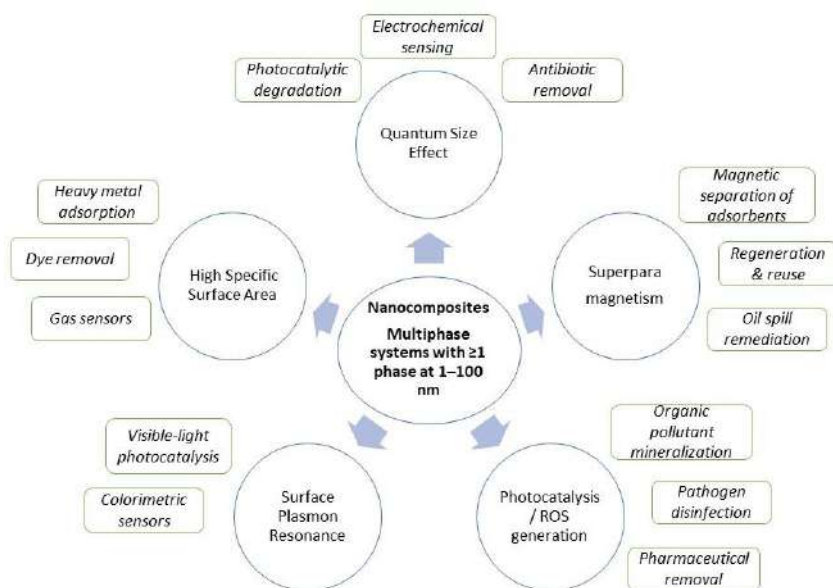


Figure 0.1. Conceptual map of the manual. Arrows connect key nanophysical mechanisms (high specific surface area, quantum size effect, superparamagnetism, photocatalysis) to concrete environmental and safety applications. [Original figure, created by the authors.]

Definition and Classification of Nanocomposites

Nanocomposites (NCs) are multiphase solid materials where at least one constituent phase has dimensions between 1 and 100 nm [5, 6]. These materials generally consist of a primary continuous phase known as the matrix (which can be polymeric, ceramic, or metallic) and a dispersed reinforcing phase referred to as the nanofiller. From a physical perspective, nanocomposites are classified based on the dimensionality of their nanoscale components [7]:

- Zero-dimensional (0D): Nanoparticles (e.g., Fe_3O_4 , TiO_2), fullerenes.
- One-dimensional (1D): Carbon nanotubes (CNTs), nanorods, nanofibers.
- Two-dimensional (2D): Graphene, graphene oxide (GO), MXenes.
- Three-dimensional (3D): Interpenetrating networks, hybrid nanograins.

The fundamental distinction of NCs compared to traditional composites is the synergistic effect that emerges from the vastly increased interfacial area between the matrix and the nanoscale

reinforcement. This high surface-to-volume ratio allows for unique physical and chemical interactions that do not exist in bulk counterparts [5].

Physical Mechanisms Driving Environmental Efficiency

- **Surface Phenomena and Porosity:** The extremely high specific surface area of NCs provides a significantly larger number of active binding sites for the adsorption of pollutants. Mechanisms such as Van der Waals forces, electrostatic interactions, and π - π stacking enable the efficient removal of heavy metals and organic dyes from wastewater [9, 10].
- **Quantum Size Effects:** As material size decreases to the nanoscale, electronic energy states become discrete, and the bandgap (E_g) can be tuned. This manipulation is vital for photocatalysis, where NCs accelerate the generation of electron-hole pairs and decrease their recombination rate, enabling the degradation of toxic organic compounds under visible or UV light [11].
- **Magnetic Susceptibility:** The integration of superparamagnetic nanoparticles (such as Fe_3O_4) into a composite matrix allows for the rapid and energy-efficient recovery of adsorbents using an external magnetic field. This solves the practical problem of separating fine particles from treated water [12].
- **Enhanced Mass Transport:** In membrane physics, the inclusion of carbon nanotubes can create aligned nano-channels that exhibit "frictionless" water transport, significantly increasing permeability while maintaining high selectivity [13].

Life Cycle Risks and Safety Concerns

While nanocomposites offer significant benefits, their entire life cycle—from raw material acquisition and manufacturing to use and final disposal—presents specific risks that must be addressed.

- **Production Burdens:** The synthesis of certain nanomaterials, such as carbon nanotubes via Chemical Vapor Deposition (CVD), is often energy-intensive and involves hazardous precursors or catalysts. This creates a "production paradox" where the early-stage environmental burden may initially outweigh the remediating benefits. (CVD synthesis of CNTs requires 1–900 MJ/kg [16])
- **Leaching and Secondary Pollution:** During the use phase, particularly in water treatment, there is a risk of nanoparticle leaching from the composite matrix. Released nanoparticles can enter the environment, potentially causing toxicity to aquatic organisms and humans through the generation of reactive oxygen species (ROS) and oxidative stress [17].
- **End-of-Life Management:** The disposal of nano-enabled products, such as filters or E-waste, lacks standardized regulatory frameworks. Improper disposal can lead to long-term persistence of nanomaterials in soil and groundwater, affecting microbial diversity and ecosystem health [18].

Chapter 1. Physics of Surface Phenomena and Dimensional Effects

1.1. Geometry and Specific Surface Area

The transition from bulk materials to the nanometric scale introduces a fundamental shift in the physical behavior of matter, primarily driven by geometric considerations. Nanomaterials are defined as having at least one dimension between 1 and 100 nm. At this scale, the physical and chemical properties of a substance are no longer determined solely by its bulk composition but are dominated by its surface characteristics. The most significant geometric consequence of downsizing is the drastic increase in the surface-to-volume ratio (S/V) [5, 9].

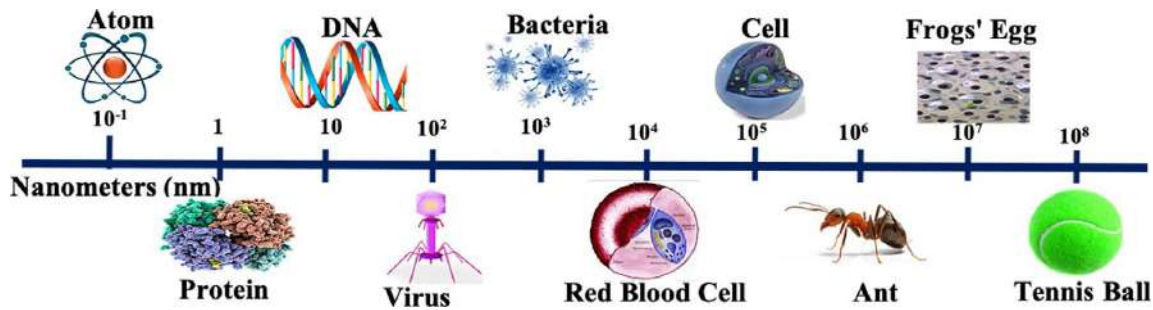


Figure 1.1. Comparison of species sizes relative to the nanometer scale, illustrating the scale at which material properties deviate from bulk behavior. [Cotica, L.F. et al. *Bionanocomposites for Wastewater Treatment*, Elsevier, 2018. Fig. 1. doi:10.1007/978-981-10-8666-3_1]

1.1.1. Mathematical Relationship: Surface-to-Volume Ratio

$$S/V = (4\pi r^2) / (4/3 \cdot \pi r^3) = 3/r$$

r — particle radius [m]; S — surface area [m²]; V — volume [m³].

As $r \rightarrow$ nanoscale (10^{-9} m), $S/V \rightarrow \infty$. For $r = 5$ nm: $S/V = 6 \times 10^8$ m⁻¹.

A large fraction of atoms are surface-located with 'dangling' bonds and high potential energy, driving increased reactivity and adsorption capacity. [9]

As the radius r approaches the nanoscale (10^{-9} m), the value of S/V increases toward infinity. Physically, this implies that a larger percentage of the material's atoms are located at the surface rather than within the interior lattice. For example, in a particle of several micrometers, the fraction of surface atoms is negligible; however, in a 10 nm particle, a significant fraction of atoms are "coordinated-unsaturated," meaning they have dangling bonds and higher potential energy.

This geometric evolution leads to dimensional effects, where the high surface energy drives increased reactivity and adsorption capacity. Furthermore, the shape (dimensionality) of the nanofiller—whether 0D (nanoparticles), 1D (nanotubes), or 2D (graphene)—further influences the available surface area.

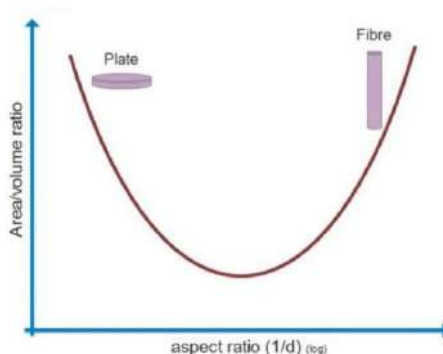


Figure 1.2. Relationship between area-to-volume ratio and particle aspect ratio: non-spherical particles (sheets, fibers) achieve even higher surface areas. [Khodakarami, M. & Bagheri, M. J. *Cleaner Production*, 2021, 296, 126404. Fig. 19a. doi:10.1016/j.jclepro.2021.126404]

1.1.2. Role of High Porosity in Creating Active Sites

In the context of environmental physics, porosity is the primary driver for creating "active sites" where pollutants can be trapped or degraded. Nanocomposites leverage their unique geometry to provide a vast network of internal surfaces.

1. **Classification of Pores:** According to IUPAC standards, porous materials are classified by their pore diameter (d):
 - o Microporous: $d < 2$ nm.
 - o Mesoporous: $2 < d < 50$ nm.
 - o Macroporous: $d > 50$ nm.
2. **Creation of Active Binding Sites:** High porosity results in a high Specific Surface Area (SSA). For instance, graphene possesses a theoretical SSA of $2630 \text{ m}^2/\text{g}$, while carbon nanotubes range from 150 to $1500 \text{ m}^2/\text{g}$ [10]. This "well-developed" porous structure provides a significantly larger number of adsorption sites compared to conventional materials like activated carbon (typically up to $1500 \text{ m}^2/\text{g}$).
3. **Capillary Filling and Mass Transport:** The geometry of these pores facilitates capillary filling, where pollutants are drawn into the internal cavities of the composite via surface tension and pressure gradients. In membrane physics, nanomaterials (like CNTs or MXenes) can create nano-channels that minimize friction, allowing for high flux rates of water while effectively sieving out contaminants through size exclusion.
4. **Stabilization in Matrices:** A key physical benefit of nanocomposites is their ability to "fix" the nanodispersed state. Free nanoparticles tend to aggregate to decrease their surface energy, which reduces their effective SSA. By embedding them in a porous matrix (e.g., polymer or ceramic), the particles are stabilized, maintaining their high porosity and active site density for long-term environmental remediation [11].

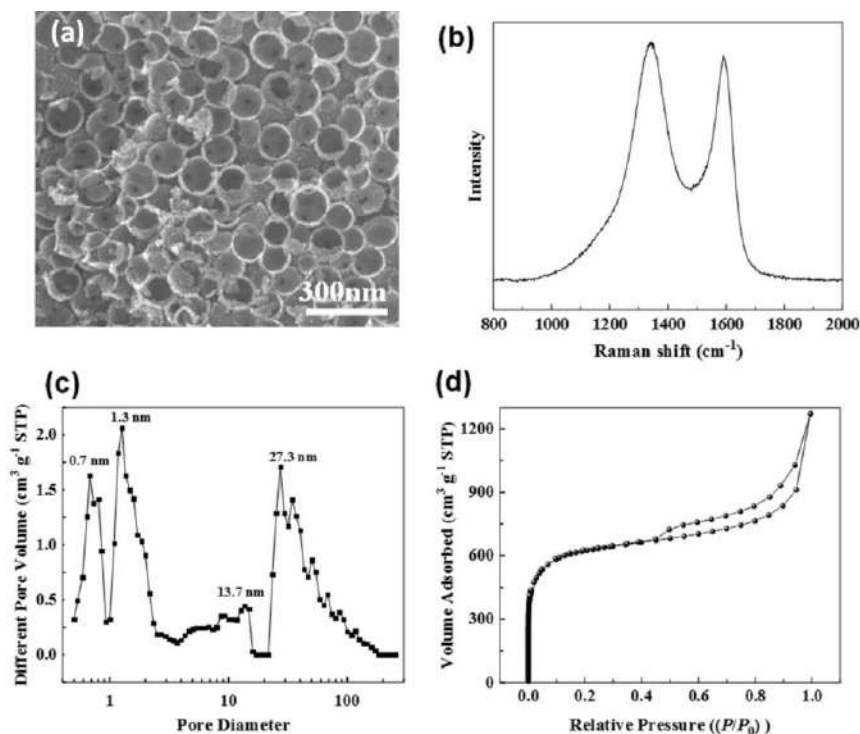


Figure 1.3. Hierarchical pore architecture and textural characteristics of a porous carbon nanocomposite, demonstrating how micro-, meso-, and macropores work together to create a high density of active sites for pollutant adsorption. The SEM image reveals a three-dimensional network of interconnected hollow carbon spheres, where intraparticle micropores ($d < 2$ nm) and mesopores ($2 < d < 50$ nm) are combined with larger interparticle macropores ($d > 50$ nm) formed by the voids between particles. The nitrogen adsorption–desorption isotherm (77 K) exhibits a steep uptake at low relative pressure (micropore filling), a pronounced hysteresis loop at intermediate P/P_0 (capillary condensation in mesopores), and a gradual increase as P/P_0 approaches 1 (contribution of macropores), confirming the presence of a hierarchical pore system. The corresponding pore-size distribution shows distinct contributions from micro-, meso-, and macropores, and the optimized material reaches a BET specific surface area above $2000 \text{ m}^2/\text{g}$, illustrating the direct link between hierarchical porosity, enlarged internal surface, and enhanced adsorption performance in environmental applications. [Cai, L.-F. et al. Structural control of a novel hierarchical porous carbon material and its adsorption properties. *Scientific Reports*, 2022, 12, 2765. Fig. 5a,c,d. doi:10.1038/s41598-022-06781-9]

1.2. Electronic Properties, Quantum Effects, and the Brus Equation

In the nanodispersed range, material properties are no longer dictated by classical physics alone; instead, they are dominated by quantum dimensional effects. These effects manifest when the physical dimensions of a particle become comparable to characteristic lengths such as the free path of charge carriers, the De Broglie wavelength, or the exciton size.

When particle dimensions approach the exciton Bohr radius, continuous energy bands split into discrete levels — the Quantum Size Effect (QSE) [11, 20]. This enables bandgap E_g tuning for photocatalytic applications.

Physics Highlight | Brus Equation: Quantitative Bandgap–Size Relationship

$$E_g(r) = E_g(\text{bulk}) + \frac{\hbar^2 \pi^2}{2r^2} \cdot \left(\frac{1}{m_e^*} + \frac{1}{m_h^*} \right) - \frac{1.8e^2}{4\pi\epsilon\epsilon_0 r}$$

where:

$E_g(r)$ — bandgap of nanoparticle of radius r [eV];

$E_g(\text{bulk})$ — bulk bandgap: TiO₂ anatase 3.2 eV; ZnO 3.37 eV; CdSe 1.74 eV;

$\hbar$ — reduced Planck constant (1.055×10^{-34} J·s);

r — nanoparticle radius [m];

m_e^*, m_h^* — effective masses of electron and hole [kg]

(TiO₂: $m_e^* \approx 9 \times 10^{-31}$ kg; $m_h^* \approx 3 \times m_e^*$);

e — elementary charge (1.6×10^{-19} C);

ϵ — relative dielectric permittivity (TiO₂: $\epsilon \approx 86$);

ϵ_0 — permittivity of free space (8.85×10^{-12} F/m).

First term (+): kinetic energy of quantum confinement → widens E_g .

Second term (−): Coulomb e^-h^+ attraction → narrows E_g .

Example (TiO₂, $r = 3$ nm): $E_g \approx 3.2 + 0.45 - 0.12 = 3.53$ eV;

absorption edge blue-shifts from 388 nm (bulk) to ~351 nm. [21]

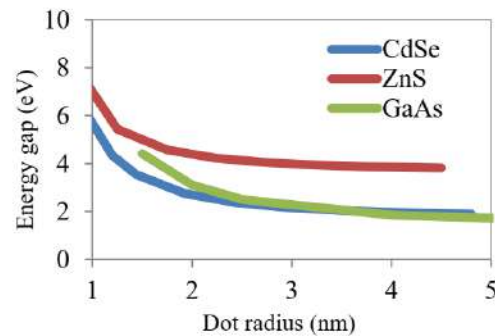


Figure 1.4. Energy gap E_g as a function of quantum dot radius r for CdSe, ZnS, and GaAs semiconductor quantum dots, calculated using the particle-in-a-box model (simplified Brus equation without the Coulomb term). As the dot radius decreases from ~5 nm to ~1 nm, E_g increases significantly above the bulk value — a direct manifestation of quantum confinement. The strong-confinement regime ($r <$ exciton Bohr radius) corresponds to the steep region of each curve. Among the three materials, CdSe shows the widest tunable range across the visible spectrum (from red at $r \approx 3.4$ nm to green at $r \approx 2.2$ nm), making it the benchmark material for quantum-confinement studies. [Onyia, A.I., Ikeri, H.I. & Nwobodo, A.N. *Theoretical study of quantum confinement effects on quantum dots using particle in a box model. Chalcogenide Letters*, 2019, 16(2), 49–57. Fig. 2. Available at: https://chalcogen.ro/49_IkeriHI.pdf]

1.2.1. Quantum Size Effect (QSE) and Environmental Utility

The Quantum Size Effect refers to the modification of the electronic structure as the particle size decreases, typically below 10–15 nm.

- **Discrete Energy Levels:** As a material reaches the nanoscale, the continuous energy bands characteristic of bulk solids split into discrete energy levels. This phenomenon is analogous to a particle in a 1D box, where the energy gap increases as the box size (particle diameter) decreases.

- **Bandgap Engineering (E_g):** In semiconductors like TiO_2 or ZnO , decreasing the particle size leads to a widening of the bandgap (E_g), often observed as a "blue shift" in optical absorption spectra. For environmental applications, this allows for precise tuning of the material to match specific light wavelengths, such as UV or visible solar radiation, for maximum photocatalytic efficiency.
- **Catalytic Reactivity:** Quantum confinement significantly influences the density of electronic states, which in turn drives catalytic properties. Smaller nanoparticles exhibit reduced recombination rates of photogenerated electron-hole pairs because the distance charge carriers must travel to reach the active surface is dramatically shortened.

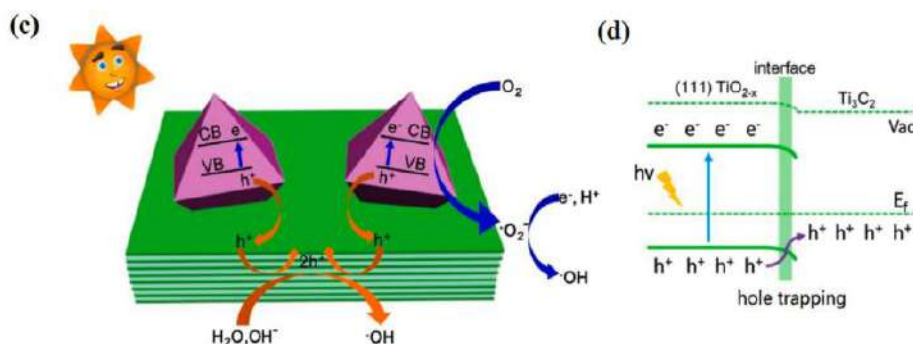


Figure 1.5. Band alignments and charge carrier mechanism in a $\text{TiO}_2/\text{Ti}_3\text{C}_2$ (MXene) nanocomposite, demonstrating how interfacial energy-level engineering enhances photoinduced carrier separation and reactive oxygen species (ROS) generation. Under solar irradiation, photons with energy $\geq E_g(\text{TiO}_2)$ create electron-hole pairs (e^-/h^+) in the TiO_2 domains; photogenerated electrons are efficiently transferred from the TiO_2 conduction band (CB) to the metallic Ti_3C_2 layers, which act as an electron sink, while the corresponding holes remain in the TiO_2 valence band (VB). This spatial separation suppresses e^-/h^+ recombination and enables interfacial redox reactions: CB electrons on Ti_3C_2 reduce dissolved O_2 to superoxide radicals ($\cdot\text{O}_2^-$) and subsequently to hydroxyl radicals ($\cdot\text{OH}$), whereas VB holes oxidize $\text{H}_2\text{O}/\text{OH}^-$ to $\cdot\text{OH}$ on the TiO_2 surface, driving the mineralization of organic pollutants. The band diagram (panel d) shows the alignment of the Fermi level (E_f) of Ti_3C_2 below the CB of TiO_2 , formation of a Schottky-like junction at the (111) $\text{TiO}_{2-x}/\text{Ti}_3\text{C}_2$ interface, downhill electron transfer from TiO_2 to MXene, and effective hole trapping in TiO_2 , together explaining the observed improvement in photocatalytic efficiency of the $\text{TiO}_2/\text{Ti}_3\text{C}_2$ nanocomposite compared to bare TiO_2 . [Bhattacharjee, B. et al. Synergistic photocatalytic degradation of dyes using $\text{TiO}_2/\text{Ti}_3\text{C}_2$ MXene nanocomposites under visible light. J. Environ. Management, 2022, 319, 115673. Fig. 2c,d. doi:10.1016/j.jenvman.2022.114673]

1.2.2. Electron Tunneling and Interfacial Charge Transfer

The performance of a nanocomposite depends heavily on the physics of the interface between the matrix and the nanofiller. Efficient charge transport across these boundaries is critical for applications such as electrochemical sensors and microbial fuel cells.

- **Physics of Heterojunctions:** When a semiconductor (like TiO_2) is paired with a conductive nanofiller (like graphene or MXenes), a Schottky barrier often forms at the interface ($\text{TiO}_2/\text{Ti}_3\text{C}_2$) due to differences in work functions [22]. This barrier acts as a directional "gate," preventing the back-flow of electrons and effectively segregating photogenerated charges, which boosts the degradation of organic pollutants.

- **Quantum Tunneling:** In composites where conductive fillers (e.g., carbon nanotubes or metal nanoparticles) are dispersed in an insulating polymer matrix, electrical conductivity often occurs via macroscopic quantum tunneling. Electrons "jump" between adjacent conductive sites even when a physical barrier exists, provided the distance is small enough (the percolation threshold) [11].
- **Vector Charge Transport:** Advanced 1D nanostructures, such as nanotubes or nanowires, facilitate vector charge transfer. Unlike spherical particles where charge moves randomly, 1D channels provide a direct pathway for electrons, significantly reducing the probability of recombination and enhancing the sensitivity of environmental monitoring devices [11].
- **Z-Scheme Systems:** Modern environmental physics employs Z-scheme photocatalytic systems, which mimic natural photosynthesis. These heterostructures use an interfacial mediator to facilitate the transfer of electrons from one semiconductor's conduction band to another's valence band, maintaining high redox potential for the degradation of persistent toxic compounds [22].

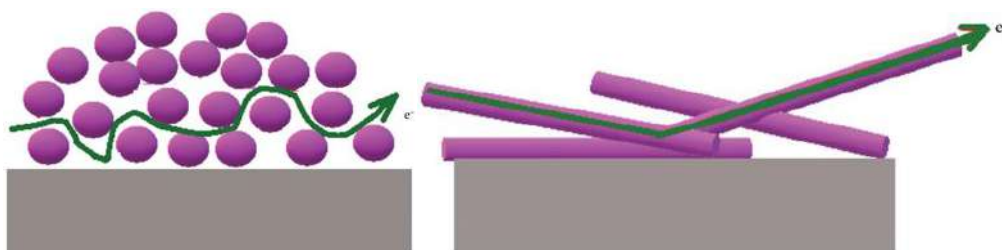


Figure 1.6. Comparison of vector charge transfer in (a) spherical nanoparticles and (b) nanotube films, illustrating how nanostructure dimensionality controls charge transport pathways in nanocomposite-based sensors and photocatalysts discussed in Chapter 1. In the case of dispersed spherical nanoparticles (a), photogenerated or injected electrons must hop randomly between isolated particles through the insulating matrix, following tortuous, multi-step trajectories with numerous potential trapping and recombination events; this geometry corresponds to the isotropic transport picture described in Section 1.2.2, where conduction is dominated by tunneling between discrete conductive islands at the percolation threshold. In contrast, aligned or percolated nanotube films (b) form quasi-one-dimensional (1D) conduction highways that guide electrons along continuous pathways from the excitation site to the current collector or reaction interface, dramatically shortening the effective transport distance and reducing the probability of encountering traps. This vector (directional) charge transfer explains why nanocomposites incorporating CNT networks or similar 1D structures exhibit higher carrier mobility, faster sensor response, and lower recombination losses in photocatalytic systems, as emphasized in the discussion of nanosensors (Section 1.4) and Z-scheme heterostructures later in the manual. [Dontsova, T.A. et al. Synthesis and Photocatalytic Properties of Nanomaterials Based on TiO_2 with Various Morphologies. *Journal of Nanomaterials*, 2019, 5942194. Fig. 13. doi:10.1155/2019/5942194]

1.3. Magnetism at the Nanoscale: Superparamagnetism and the Néel–Arrhenius

Law

The magnetic behavior of matter undergoes a qualitative transformation when dimensions are reduced below a critical threshold, typically referred to as the single-domain limit ($\sim 20\text{--}50$ nm for iron oxides). For materials such as magnetite (Fe_3O_4), this transition allows for the manifestation of superparamagnetism, a physical state that is highly sought after for environmental engineering

because it combines the strong magnetic response of ferromagnets with the lack of magnetic remanence characteristic of paramagnets [12, 23].

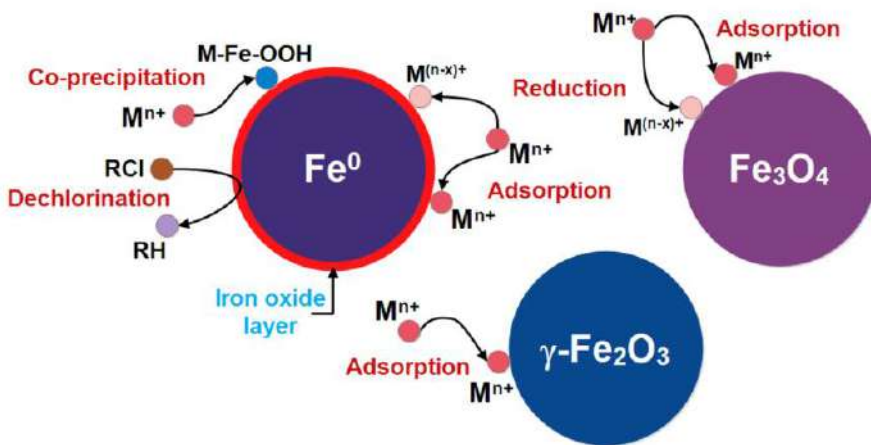


Figure 1.7. Contaminant removal by three iron-based nanoparticles – zero-valent iron (ZVI), magnetite (Fe₃O₄), and maghemite (γ-Fe₂O₃) – illustrating how differences in surface chemistry, oxidation state, and magnetic properties govern interfacial interactions with pollutants, as discussed in Sections 1.1, 1.3 and Chapter 2 of this manual. The schematic shows that ZVI nanoparticles primarily remove contaminants via simultaneous reductive transformation and adsorption: the Fe⁰ core donates electrons to reducible species (e.g. Cr(VI), nitroaromatics), while the corrosion products (Fe(II)/Fe(III) (oxy)hydroxides) formed on the shell provide fresh hydroxylated surfaces and inner-sphere complexation sites for heavy metal cations. In contrast, Fe₃O₄ and γ-Fe₂O₃ nanoparticles act predominantly as high-surface-area adsorbents, where surface –OH groups are protonated/deprotonated depending on pH, enabling electrostatic attraction, complexation, and co-precipitation of metal ions and dyes, in full agreement with the pH- and speciation-dependent sorption mechanisms described in Section 2.1. At the same time, all three iron oxides are superparamagnetic in the nanometric size range considered here, so that after loading with pollutants they can be rapidly separated from water by an external magnetic field and subsequently regenerated, directly illustrating the “separation paradox” and its solution via magnetic nanocomposites analyzed in Section 1.3. By juxtaposing ZVI, Fe₃O₄, and γ-Fe₂O₃ in a single panel, the figure visually connects the geometric and surface concepts of high specific surface area (Section 1.1.1), the magnetic behavior at the nanoscale (Néel–Arrhenius law and blocking temperature, Section 1.3), and the sorption thermodynamics and kinetics of Chapter 2 into one coherent picture of how iron-based nanocomposites function as efficient, magnetically recoverable adsorbents in environmental remediation. [Khodakarami, M. & Bagheri, M. Recent advances in synthesis and application of polymer nanocomposites for water and wastewater treatment. *Journal of Cleaner Production*, 2021, 296, 126404. Fig. 15. doi:10.1016/j.jclepro.2021.126404]

1.3.1. Physical Justification of Magnetic Susceptibility

In bulk ferromagnetic or ferrimagnetic materials, the structure is divided into multiple magnetic domains to minimize magnetostatic energy. However, as the particle size decreases (typically below 20–50 nm for iron oxides), the energy required to create a domain wall becomes greater than the energy of the single-domain state.

- **Thermal Fluctuations and Energy Barriers:** In these single-domain nanoparticles, the magnetic moment of the entire particle can be viewed as one giant spin. The energy required to flip this spin is determined by the anisotropy energy barrier (KV , where K is the anisotropy constant and

V is the volume). When the thermal energy ($k_B T$) exceeds this barrier, the magnetic moments flip randomly, leading to a net magnetization of zero in the absence of a field.

- **Langevin Behavior:** When an external magnetic field is applied, these giant spins align rapidly with the field. Physically, this results in a very high magnetic susceptibility. Unlike bulk materials, superparamagnetic nanoparticles exhibit zero coercivity and zero remanence, meaning they do not retain magnetism once the external field is removed.
- **Minimized Energy Loss:** In superparamagnetic systems, losses associated with the absorption and release of magnetic energy (hysteresis) are minimized, making them efficient contrast agents and controllable carriers.

Physics Highlight | Néel–Arrhenius Equation and Blocking Temperature T_B

Relaxation time of the magnetic moment of a single-domain nanoparticle [23]:

$$\tau = \tau_0 \cdot \exp(K \cdot V / k_B \cdot T)$$

where:

τ — thermal relaxation time [s] (mean interval between spontaneous reversals);

τ_0 — attempt frequency pre-factor ($\tau_0 \approx 10^{-9}$ – 10^{-12} s for ferrites);

K — uniaxial magnetic anisotropy constant [J/m^3]

(Fe_3O_4 : $K \approx 11 \text{ kJ}/\text{m}^3$; CoFe_2O_4 : $K \approx 200 \text{ kJ}/\text{m}^3$);

V — particle volume [m^3];

k_B — Boltzmann constant ($1.38 \times 10^{-23} \text{ J/K}$);

T — absolute temperature [K].

Blocking temperature T_B (from condition $\tau = \tau_m$, measurement time):

$$T_B = K \cdot V / (k_B \cdot \ln(\tau_m / \tau_0))$$

$\tau_m \approx 100 \text{ s}$ (DC SQUID magnetometry); $\ln(\tau_m/\tau_0) \approx 25$ for $\tau_0 = 10^{-9} \text{ s}$.

Numerical example for Fe_3O_4 nanoparticles ($K = 11 \text{ kJ}/\text{m}^3$, $d = 10 \text{ nm}$, $\tau_0 = 10^{-9} \text{ s}$):

$V = \pi/6 \cdot (10 \times 10^{-9})^3 \approx 5.24 \times 10^{-25} \text{ m}^3$;

$T_B \approx (11 \times 10^3 \times 5.24 \times 10^{-25}) / (1.38 \times 10^{-23} \times 25) \approx 16.6 \text{ K}$.

→ Fe_3O_4 particles with $d \leq 10 \text{ nm}$ are superparamagnetic at room temperature ($T \gg T_B$).

For $d = 20 \text{ nm}$ (V increased 8×): $T_B \approx 133 \text{ K}$ — still superparamagnetic at RT.

For $d = 30 \text{ nm}$: $T_B \approx 450 \text{ K}$ — becomes ferrimagnetic at RT. [23]

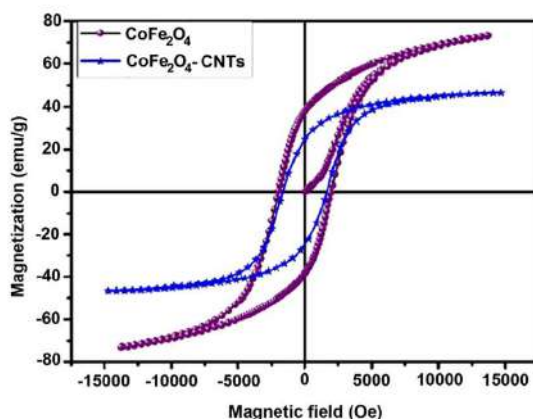


Figure 1.8. Magnetic hysteresis loops of CoFe_2O_4 nanoparticles and $\text{CoFe}_2\text{O}_4/\text{CNT}$ nanocomposites, showing that incorporation of CNTs narrows the loop and reduces coercivity H_c and remanent magnetization M_r . This behavior indicates easier thermally activated reversal of magnetic moments and a shift toward superparamagnetic-like behavior, as discussed in Section 1.3 through the Néel–Arrhenius law and the concept of blocking temperature. For the logic of the manual, the figure is important because it provides an experimental illustration of why magnetic nanocomposites can be efficiently collected by an external field yet remain easy to redisperse and regenerate after field removal, which is essential for reusable adsorbents in water purification. [Routray, K.L. et al. Synthesis and characterization of $\text{CoFe}_2\text{O}_4/\text{MWCNTs}$ nanocomposites and investigation of their magnetic properties. *Materials Science and Engineering: B*, 2017, 226, 199–205. doi:10.1016/j.mseb.2017.09.021]

1.3.2. Mechanisms of Magnetic Separation in Water Purification

The integration of magnetic nanoparticles into composites addresses the "separation paradox" in nanotechnology: while smaller particles are more efficient at adsorbing pollutants, they are significantly harder to remove from water using traditional filtration.

- **Magnetic Separation (MS) and Recovery:** The primary physical mechanism is the use of an external magnetic field gradient to pull the pollutant-laden magnetic nanocomposites out of the treated water stream. This process is rapid, cost-effective, and prevents the "breakthrough" of fine particles into the treated water [12].
- **High-Gradient Magnetic Separation (HGMS):** For industrial applications, HGMS utilizes specialized filters with high magnetic gradients to capture even very small magnetic particles (MNPs) functionalized with specific ligands (e.g., dithiocarbamate for mercury removal) [24].
- **Selective Targeted Capture:** By engineering the surface of the magnetic core with functional groups (chitosan, polymers, or silica), the composite can selectively bind to specific ions (e.g., Pb^{2+} , $\text{As}^{3+/5+}$) or pathogens through electrostatic interactions and chelation before being physically removed by a magnet [12, 24].
- **Regeneration and Reusability:** Because these materials are superparamagnetic, they can be easily "de-magnetized" simply by removing the external field, allowing for the easy release of the adsorbent for chemical regeneration and reuse for >10 cycles [12].

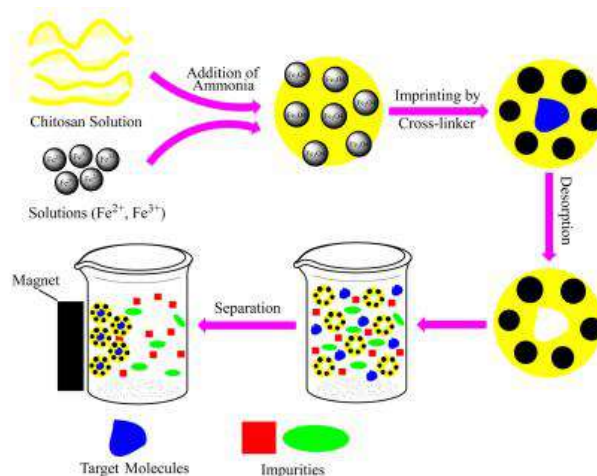


Figure 1.9. Complete adsorption–magnetic separation–regeneration cycle using Calcon-imprinted magnetic chitosan (CIMC) nanoparticles, illustrating the operating principle of reusable magnetic nanocomposite adsorbents for dye removal from water. The scheme shows selective adsorption of dye molecules on the chitosan-based surface, magnetic recovery of the loaded particles by an external field, and desorption/regeneration before reuse in the next cycle. In the context of the manual, this figure directly supports Section 1.3.2, where magnetic nanocomposites are presented as a solution to the separation paradox: they preserve the high surface area and adsorption efficiency of nanosized sorbents while enabling rapid and simple recovery from water. It also connects with Chapter 2, since the chitosan shell provides the functional groups responsible for selective interfacial binding of dye molecules, whereas the regeneration step emphasizes reusability and reduction of secondary waste in environmental remediation. [Gulati, S. et al. Recent progress, synthesis, and application of chitosan-decorated magnetic nanocomposites in remediation of dye-laden wastewaters. *New Journal of Chemistry*, 2022, 46, 17114–17139. Fig. 11. doi:10.1039/D2NJ03558H]

1.4. Physics of Nanosensors for Environmental Monitoring

Nanocomposite sensors extend the manual's scope from remediation to real-time environmental monitoring — an equally critical aspect of ecological safety [25, 26]. The same nanophysical principles that drive adsorption and photocatalysis (high SSA, quantum confinement, charge transfer) are harnessed here to detect trace concentrations of pollutants.

1.4.1. Resistive Gas Sensors

Resistive nanocomposite gas sensors (e.g., ZnO/graphene, SnO₂/CNT) detect air pollutants (NO₂, NH₃, CO, VOCs) through a change in electrical resistance upon analyte adsorption [25]. Adsorption of gas molecules induces charge transfer at the nanocomposite surface → change in carrier concentration → change in resistance.

$$S = (R_0 - R_g) / R_0 \times 100\%$$

S — relative sensor sensitivity [%];

*R*₀ — baseline resistance in clean air [Ω];

*R*_g — resistance in the presence of the analyte gas [Ω].

Due to SSA > 100 m²/g, sensitivity in ZnO/graphene composites is 100–1000× higher than in microstructured analogues at the same analyte concentration. [25]

1.4.2. Electrochemical Sensors for Heavy Metals

Differential pulse voltammetry (DPV) with nanocomposite-modified electrodes (GO/Bi, MXene/Nafion) achieves ultra-low detection limits for Pb^{2+} , Cd^{2+} , and As^{3+} in drinking water [26].

$$\text{LOD} = 3 \cdot \sigma_{\text{blank}} / S_{\text{electrode}}$$

LOD — limit of detection [$\mu\text{g/L}$ or mol/L];

σ_{blank} — standard deviation of the blank signal [μA];

$S_{\text{electrode}}$ — slope of the calibration curve [$\mu\text{A} \cdot \text{L}/\mu\text{g}$].

Nanocomposite electrodes (GO/Bi, MXene/Nafion) achieve $\text{LOD}(\text{Pb}^{2+}) \approx 0.01\text{--}0.1 \mu\text{g/L}$, well below the WHO guideline of $10 \mu\text{g/L}$ for drinking water. [26]

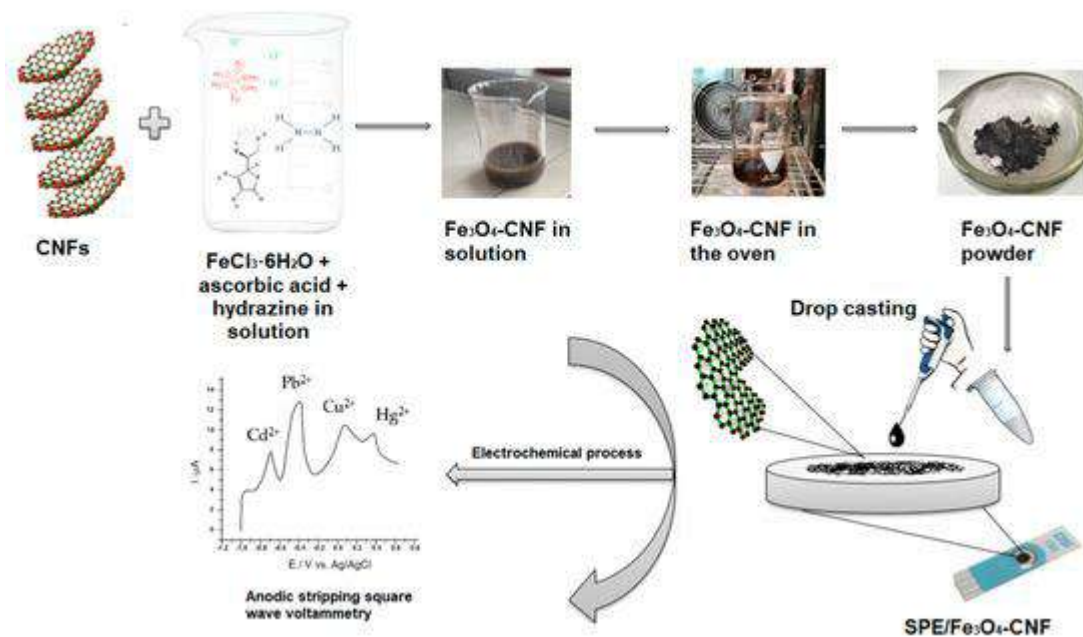


Figure 1.10 Schematic of the fabrication and operation of the SPE/Fe₃O₄-CNF electrochemical sensor for simultaneous heavy metal detection, illustrating how nanocomposite architecture is translated into a practical analytical device as discussed in Section 1.4 of this manual. The left panel shows the synthesis of the Fe₃O₄/carbon nanofiber (CNF) nanocomposite, where superparamagnetic Fe₃O₄ nanoparticles are immobilized on a conductive CNF scaffold, combining a high density of adsorption/accumulation sites with an efficient one-dimensional electron transport network. The central panel depicts the drop-casting of this nanocomposite ink onto a disposable screen-printed electrode (SPE), forming a thin, nanostructured sensing layer that increases the electroactive surface area and enhances preconcentration of target metal ions from solution. The bottom panel presents a typical anodic stripping square-wave voltammogram, in which well-resolved current peaks for Cd²⁺, Pb²⁺, Cu²⁺, and Hg²⁺ reflect the separate stripping of each metal from the modified electrode surface; peak height is directly related to the amount of metal preconcentrated, providing the analytical signal. [Dinu, A. et al. Fe₃O₄-Carbon Nanofiber Nanocomposite-Modified Screen-Printed Electrodes for Simultaneous Electrochemical Detection of Cd²⁺, Pb²⁺, Cu²⁺, and Hg²⁺ in Water Samples. *Nanomaterials*, 2024, 14(8), 702. Fig. 1. doi:10.3390/nano14080702]

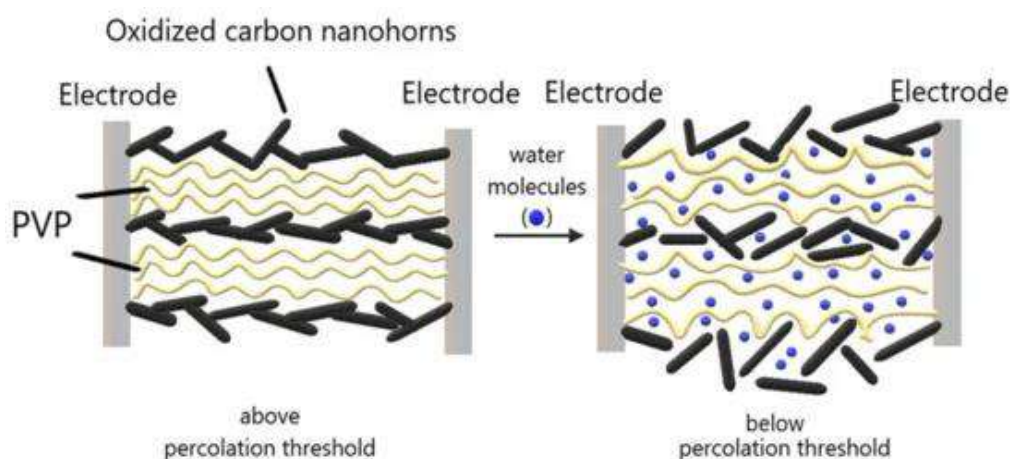


Figure 1.11. Schematic illustration of the relative humidity (RH) sensing mechanism in a PVP/CNHox resistive nanocomposite deposited on interdigitated transducer (IDT) electrodes: (left) at CNHox concentration above the percolation threshold ψ_c , a continuous conductive network of oxidized carbon nanohorns spans the inter-electrode gap, resulting in low electrical resistance; (right) upon water vapor absorption, the hygroscopic PVP matrix swells, increasing the inter-nanohorn tunneling distances and breaking percolating paths — the nanocomposite transitions to a high-resistance (below-percolation) state. The key design principle exploited here is that maximum sensitivity is achieved when the CNHox loading is set only slightly above ψ_c : even a small degree of PVP swelling is sufficient to disrupt the percolating network and cause a dramatic increase in resistance, which constitutes the transduction signal. In the context of this manual, the figure complements the discussion in Section 1.3 on how the electrical percolation threshold of a nanocomposite is not merely a structural parameter but the central design variable for high-sensitivity resistive gas and vapor sensors — illustrating how the interplay between the conductive filler geometry, polymer swelling, and IDT electrode spacing governs both the sensitivity and operating range of the sensing device. [Serban, B.-C. et al. Electrical Percolation Threshold and Size Effects in Polyvinylpyrrolidone-Oxidized Single-Wall Carbon Nanohorn Nanocomposite: The Impact for Relative Humidity Resistive Sensors Design. *Sensors*, 2021, 21(4), 1435, Fig. 9. doi:10.3390/s21041435]

1.4.3. Why Nanocomposites Outperform Conventional Sensors

The superior performance of nanocomposite-based sensors over their conventional (bulk or microstructured) counterparts is not accidental — it follows directly from the same nanophysical principles discussed in Sections 1.1 and 1.2. Table 1.1 summarizes the key physical advantages.

<i>Physical parameter</i>	<i>Conventional sensor</i>	<i>Nanocomposite sensor</i>	<i>Physical reason</i>
<i>Specific surface area</i>	<i>$\sim 1\text{--}10\text{ m}^2/\text{g}$</i>	<i>$100\text{--}2630\text{ m}^2/\text{g}$</i>	<i>$S/V = 3/r \rightarrow$ more analyte binding sites</i>
<i>Response time</i>	<i>minutes</i>	<i>seconds</i>	<i>shorter diffusion path to active surface</i>
<i>Operating temperature</i>	<i>$200\text{--}400\text{ }^\circ\text{C}$</i>	<i>room temperature</i>	<i>high surface reactivity compensates for low T</i>
<i>LOD for heavy metals</i>	<i>$\sim 10\text{ }\mu\text{g/L}$</i>	<i>$0.01\text{--}0.1\text{ }\mu\text{g/L}$</i>	<i>nanocomposite electrode amplifies signal</i>
<i>Selectivity</i>	<i>low (cross-sensitivity)</i>	<i>high (tunable surface chemistry)</i>	<i>functional groups engineered per target analyte</i>

Chapter 2. Physics of Sorption Processes and Membrane Purification

This chapter analyzes the physical interactions and transport phenomena governing contaminant removal using nanocomposite systems [9, 27, 28].

2.1. Mechanisms of Contaminant Nanosorption and Adsorption Isotherms

Adsorption at the nanoscale is a complex surface phenomenon where pollutants (adsorbates) are concentrated at the interface of a solid nanocomposite (adsorbent). Physically, this process is governed by the balance of long-range and short-range molecular forces.

2.1.1. Physical Interactions

Nanocomposites, particularly those utilizing carbon nanomaterials like Carbon Nanotubes (CNTs) and Graphene Oxide (GO), leverage specific physical mechanisms for high-efficiency capture:

- **Van der Waals Forces and Physisorption:** These represent weak, non-specific attractive forces (dipole-dipole or induced dipole) that allow pollutants to adhere to the high-surface-area scaffolds of the matrix [9].
- **Electrostatic Interactions:** The surface charge of the nanocomposite, often determined by the solution pH relative to the material's Point of Zero Charge (PZC), dictates the attraction or repulsion of ionic species. For example, SWCNTs and MWCNTs typically carry a negative charge at pH values above 3, facilitating the capture of positively charged metal cations or cationic dyes [27].
- **π - π Stacking:** In carbon-based nanostructures, the sp^2 -hybridized carbon atoms form a delocalized π -electron system. This allows for extremely strong physical associations with organic molecules containing aromatic rings (such as dyes or pesticides) through the overlap of π -orbitals [10].

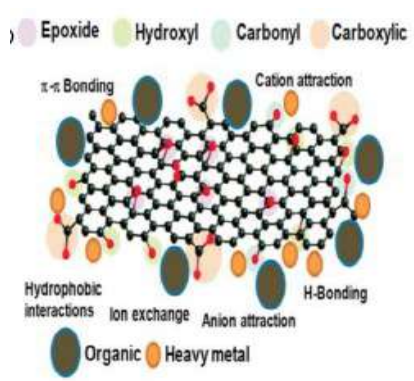


Figure 2.1. Adsorption mechanisms between graphene/graphene oxide (GO) and various contaminants: schematic representation of three dominant interaction modes — (i) functional-group interactions, where oxygen-containing groups on GO sheets (such as $-\text{COOH}$, $-\text{OH}$, $-\text{C}=\text{O}$, and epoxy) form hydrogen bonds and coordinate complexes with metal cations and polar organic molecules; (ii) electrostatic attraction between charged pollutant species and the pH-dependent surface charge of GO (negatively charged at neutral–alkaline pH, enabling binding of cationic dyes and metal ions, while surface protonation at low pH favors anion uptake via specific interactions); and (iii) π - π orbital overlap between the delocalized π -system of sp^2 -hybridized graphene domains and aromatic contaminants, which

drives strong adsorption of dyes, pharmaceuticals, and other π -conjugated organics. In the context of this manual, the figure provides the microscopic basis for Section 2.1, where the high adsorption capacity of graphene-based nanocomposites is linked to the combination of large specific surface area and multiple, tunable interaction pathways, explaining why grafting GO onto polymer, metal oxide, or bio-based supports is an effective strategy for designing multifunctional sorbents for water and wastewater treatment. [Shirsat, S.D. et al. Metal Oxide Nanocomposites in Water and Wastewater Treatment. Elsevier, 2021, Fig. 14.6B]

2.1.2. Influence of Thermodynamics and pH on Heavy Metal Capture

The efficiency of metal ion sequestration is highly sensitive to the thermodynamic state of the system and the electrochemical environment:

- **Role of pH:** The solution pH controls the protonation/deprotonation of functional groups (e.g., carboxyl -COOH or hydroxyl -OH) on the composite surface. At low pH, high H^+ concentration leads to surface protonation, creating a positive charge that repels metal cations but attracts anionic pollutants. Conversely, higher pH levels facilitate deprotonation, increasing the density of negative sites for the chelation of heavy metals like Pb^{2+} , Cu^{2+} , Cd^{2+} [27, 28].
- **Thermodynamic Parameters:** Adsorption can be either endothermic (capacity increases with temperature) or exothermic (capacity decreases with temperature). Endothermic systems often involve the "inflation" of the internal structure of the composite, providing easier access for contaminants to the internal pores.

2.2. Nanofluidics and Membrane Transport

Nanocomposite membranes represent a shift from passive sieving to active, high-flux separation. Transport physics at the nanoscale often defies classical macroscale fluid dynamics [13, 31].

2.2.1. "Frictionless" Water Transport in Carbon Nanotubes

One of the most remarkable phenomena in nanofluidics is the ultra-fast transport of water through the sub-nanometer channels of aligned CNTs.

- **Physical Basis:** The atomic smoothness of the hydrophobic graphitic walls minimizes the frictional resistance for water molecules. Water molecules tend to form ordered, "wire-like" chains within these nano-confinements, leading to permeability rates that are several orders of magnitude higher than those predicted by the classical Hagen-Poiseuille equation.

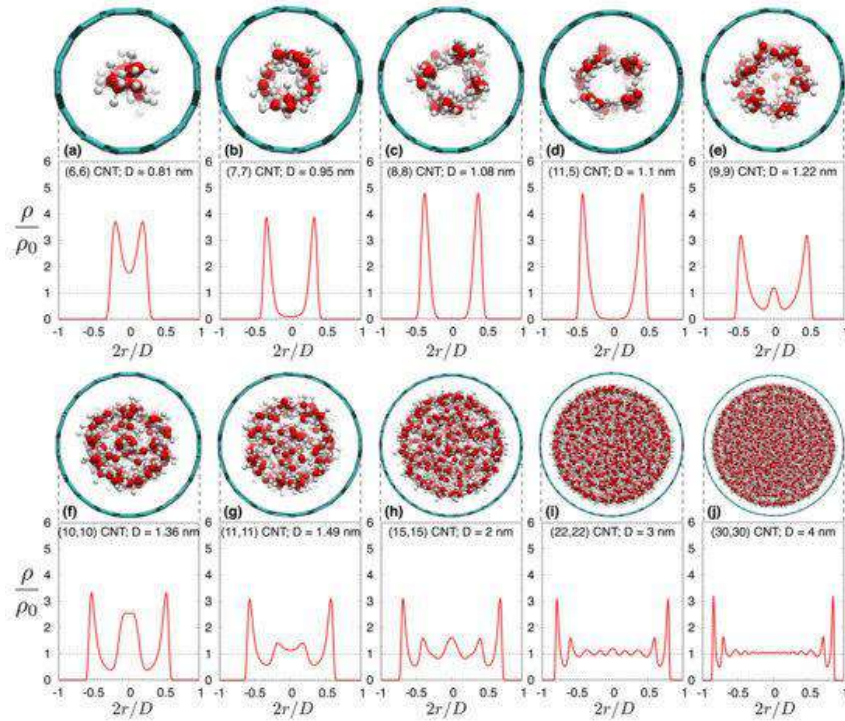


Figure 2.2 Molecular dynamics (MD) simulation snapshots of water structure inside single-walled carbon nanotubes (SWCNTs) of increasing diameter: (a) $d < 0.9$ nm — a single-file chain of hydrogen-bonded water molecules oriented along the tube axis; (b) $d \approx 1.0$ – 1.2 nm — transition to a double-helical arrangement; (c) $d > 1.5$ nm — concentric cylindrical rings of water molecules. The single-file regime (a) is the physical origin of ultra-fast water transport: the cooperative, burst-like motion of the hydrogen-bond chain proceeds with near-zero friction against the atomically smooth hydrophobic graphene wall, producing flow rates 3–4 orders of magnitude larger than predicted by the Hagen–Poiseuille equation for the same pressure gradient. This behavior has no analogue in macroscale fluid dynamics and forms the physical basis for the high permeability of CNT-composite membranes discussed in Section 2.2 of this manual, where these nanoscale transport features are linked to the design of low-pressure, high-flux nanocomposite membranes for water purification. [Chatzichristos, A. & Hassan, J. Nanoscale water transport and structure inside carbon nanotubes: a molecular dynamics study. *Nanomaterials*, 2022, 12(1), 174. Fig. 4. doi:10.3390/nano12010174]

Physics Highlight | Hagen–Poiseuille Equation and Deviation in CNT Channels

Classical laminar flow in a cylindrical channel [13, 31]:

$$Q = (\pi \cdot r^4 \cdot \Delta P) / (8 \cdot \eta \cdot L)$$

where:

- Q — volumetric flow rate [m^3/s];
- r — channel radius [m];
- ΔP — pressure drop across the channel [Pa];
- η — dynamic viscosity of water ($\eta \approx 10^{-3}$ Pa·s at 20°C);
- L — channel length [m].

Key experimental result (Holt et al., *Science*, 2006 [13]):

For CNTs with inner diameter $d < 2$ nm, measured water flux exceeds Hagen–Poiseuille

prediction by 3–4 orders of magnitude. The effective slip length b can be defined:

$$Q_{\text{CNT}} = Q_{\text{HP}} \cdot (1 + 4b/r)$$

b — slip length [nm]; for CNTs $b \approx 30\text{--}500 \text{ nm} \gg r \rightarrow$ ultra-fast transport.

Physical reason: atomically smooth graphitic walls eliminate the no-slip boundary condition; water molecules form cooperative 'single-file' chains within the CNT.

Consequence for membranes: CNT-embedded polymer membranes achieve water permeability $\sim 10\text{--}100\times$ higher than conventional RO membranes at the same selectivity. [13]

2.2.2. Size Exclusion and Donnan Effect

Nanocomposite membranes utilize two primary physical mechanisms for selectivity:

- **Size Exclusion** (Sieving): Species are rejected based on the ratio between their hydrated diameter and the membrane's pore diameter.
- **Donnan Exclusion**: This is an electrostatic mechanism where a charged membrane surface repels ions of the same charge (co-ions). This effect is particularly important for removing multivalent ions from water at low operating pressures.

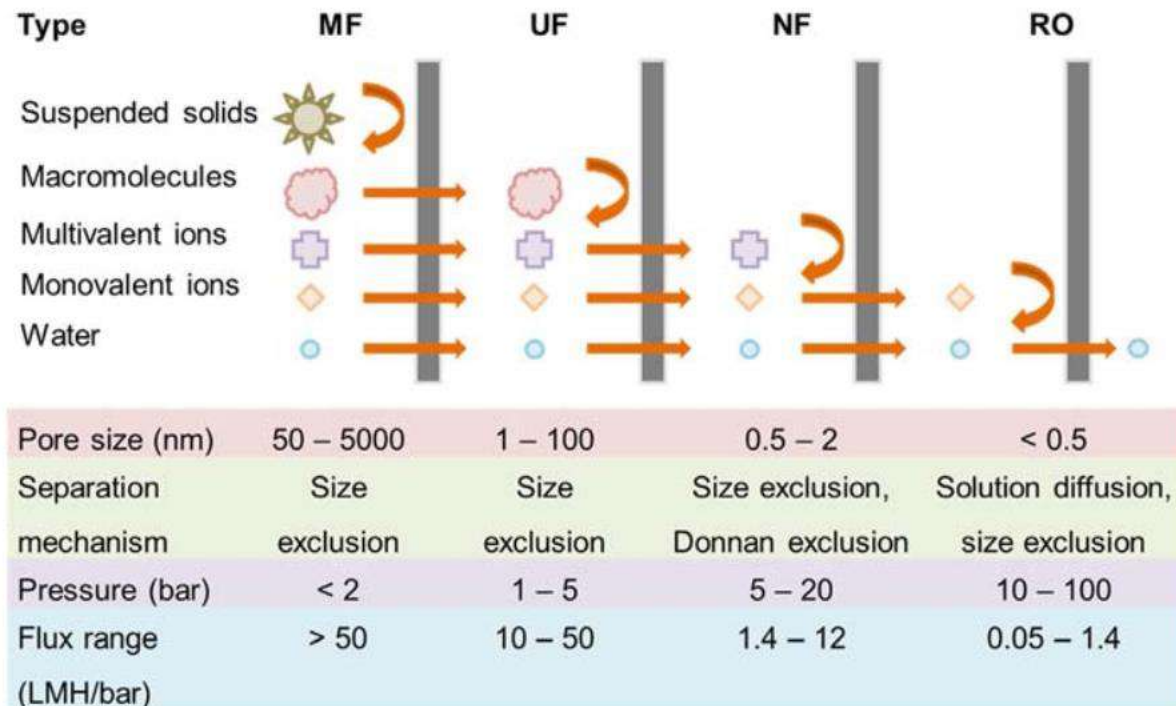


Figure 2.3. Schematic overview of pressure-driven membrane processes—microfiltration (MF), ultrafiltration (UF), nanofiltration (NF), and reverse osmosis (RO)—showing typical pore-size ranges for each membrane class and the corresponding size scales of common contaminants (suspended solids, bacteria, viruses, organic dyes, multivalent ions, and monovalent salts). The diagram illustrates how increasing transmembrane pressure and decreasing effective pore

size shift the dominant separation mechanism from simple size exclusion in MF/UF (removal of particulates and microorganisms) to a combination of sieving and electrostatic (Donnan) effects in NF (removal of multivalent ions and large organics) and finally to solution–diffusion in RO (desalination and removal of small neutral molecules). In the context of this manual, the figure provides a framework for Section 2.2 by positioning nanocomposite membranes within the broader family of pressure-driven processes: CNT- and MXene-based layers are typically engineered in the UF–NF regime, where their nanoscale channels, high specific surface area, and surface charge allow simultaneous enhancement of water flux and selectivity for targeted pollutants. [Khodakarami, M. & Bagheri, M. Recent advances in synthesis and application of polymer nanocomposites for water and wastewater treatment. *Journal of Cleaner Production*, 2021, 296, 126404. Fig. 20.3. doi:10.1016/j.jclepro.2021.126404]

Physics Highlight | Donnan Potential at a Charged Nanocomposite Membrane

The Donnan potential $\Delta\phi_{\text{Don}}$ at the charged membrane–solution interface [32]:

$$\Delta\phi_{\text{Don}} = (R \cdot T) / (z_i \cdot F) \cdot \ln(a_i^{\text{m}} / a_i^{\text{s}})$$

where:

$\Delta\phi_{\text{Don}}$ — Donnan equilibrium potential [V];

R — gas constant (8.314 J/(mol·K));

T — absolute temperature [K];

z_i — charge number of ion i (+2 for Cu^{2+} ; −1 for Cl^- ; −3 for PO_4^{3-});

F — Faraday constant (96485 C/mol);

a_i^{m} — activity of ion i in the membrane phase [mol/L];

a_i^{s} — activity of ion i in the bulk solution [mol/L].

Physical consequence: a negatively charged GO or carboxyl-CNT membrane repels anions (co-ions with same sign as membrane charge), enabling selective removal of nitrates, phosphates, and As(V) from water.

Tuning pH changes the degree of ionization of $-\text{COOH}$ and $-\text{OH}$ groups on the membrane surface, thereby controlling selectivity. [32]

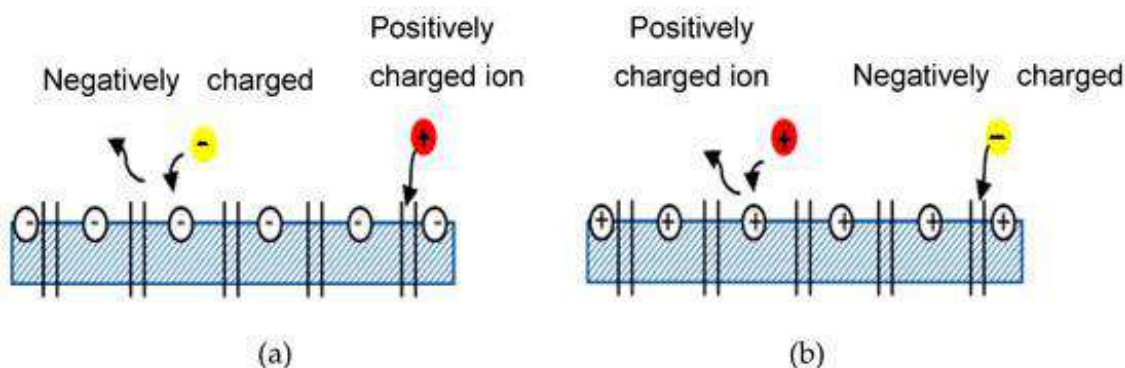


Figure 2.4 Donnan exclusion mechanism at a charged nanofiltration membrane–electrolyte solution interface: (a) negatively charged membrane (e.g., GO/polymer nanocomposite with surface $-\text{COOH}$ and $-\text{SO}_3\text{H}$ groups), where co-ions (Cl^- , SO_4^{2-}) are electrostatically repelled by fixed negative charges and cannot partition into the membrane, while counter-ions (Na^+ , Ca^{2+}) are enriched in the membrane phase and can pass through; (b) positively charged membrane, where the selectivity is reversed and cations become co-ions that are now excluded. The Donnan potential $\Delta\phi_{\text{Don}}$ at the membrane–solution interface is the thermodynamic origin of this selectivity, building up until the electrochemical potential of each ion species is equal on both sides of the interface. For a monovalent 1:1 electrolyte

such as NaCl, co-ion rejection increases as external salt concentration decreases, because the Debye screening length κ^{-1} grows and the electrostatic exclusion zone extends further into the solution; this explains why GO-based nanocomposite membranes show superior performance over conventional NF membranes when separating trace heavy metals and oxyanions at sub-millimolar concentrations, as emphasized in Section 2.2 of this manual. [Suhaimi, N.S. et al. Donnan Exclusion in Graphene Oxide-Based Nanocomposite Membranes for Ion Separation. *Nanomaterials*, 2022, 12(3), 437. Fig. 5. doi:10.3390/nano12030437]

2.3. Physics of Wettability and Oil Spill Remediation

The management of oil–water emulsions relies on controlling the contact angle (θ) at the liquid–solid interface [33, 34].

- **Superhydrophobic and Superoleophilic Surfaces:** To remediate oil spills, nanocomposites are engineered to have a water contact angle $\theta_{\text{water}} > 150^\circ$ (superhydrophobic) while maintaining a high affinity for hydrocarbons (superoleophilic) [33, 34].
- **Roughness and Hierarchical Structures:** Physical surface modification, such as adding SiO₂ or TiO₂ nanoparticles to a polymer matrix, creates a hierarchical roughness that traps air pockets. This reduces the adhesion force of water droplets, allowing oil to selectively permeate through the composite while repelling water.
- **Magnetic Recovery:** By integrating superparamagnetic iron oxide (Fe₃O₄) nanoparticles into these super-wetting matrices, the oil-soaked composite can be easily recovered from the water surface using an external magnetic field, ensuring both safety and recyclability [34].

Physics Highlight | Young Equation, Wenzel Model, and Cassie–Baxter State

Contact angle on an ideal flat surface — Young's equation [33]:

$$\cos(\theta_Y) = (\gamma_{SV} - \gamma_{SL}) / \gamma_{LV}$$

where:

γ_{SV} — solid–vapour interfacial energy [J/m²];

γ_{SL} — solid–liquid interfacial energy [J/m²];

γ_{LV} — liquid–vapour surface tension [J/m²].

Wenzel model (rough surface, fully wetted) [33]:

$$\cos(\theta_W) = r \cdot \cos(\theta_Y)$$

$r > 1$ — roughness factor (actual / projected surface area).

Roughness amplifies inherent wettability: if $\theta_Y < 90^\circ \rightarrow$ more hydrophilic;

if $\theta_Y > 90^\circ \rightarrow$ more hydrophobic.

Cassie–Baxter model (air-trapping heterogeneous state) [34]:

$$\cos(\theta_{CB}) = f_s \cdot (\cos(\theta_Y) + 1) - 1$$

f_s — fraction of surface in contact with liquid ($0 < f_s < 1$).

As $f_s \rightarrow 0$: $\cos(\theta_{CB}) \rightarrow -1$, $\theta_{CB} \rightarrow 180^\circ \rightarrow$ perfect superhydrophobicity.

For SiO₂/polymer nanocomposite surfaces, hierarchical roughness and low γ_{SV} (fluoropolymer coating) combine to achieve $\theta_{\text{water}} > 155^\circ$ while $\theta_{\text{oil}} \approx 0^\circ$. [34]

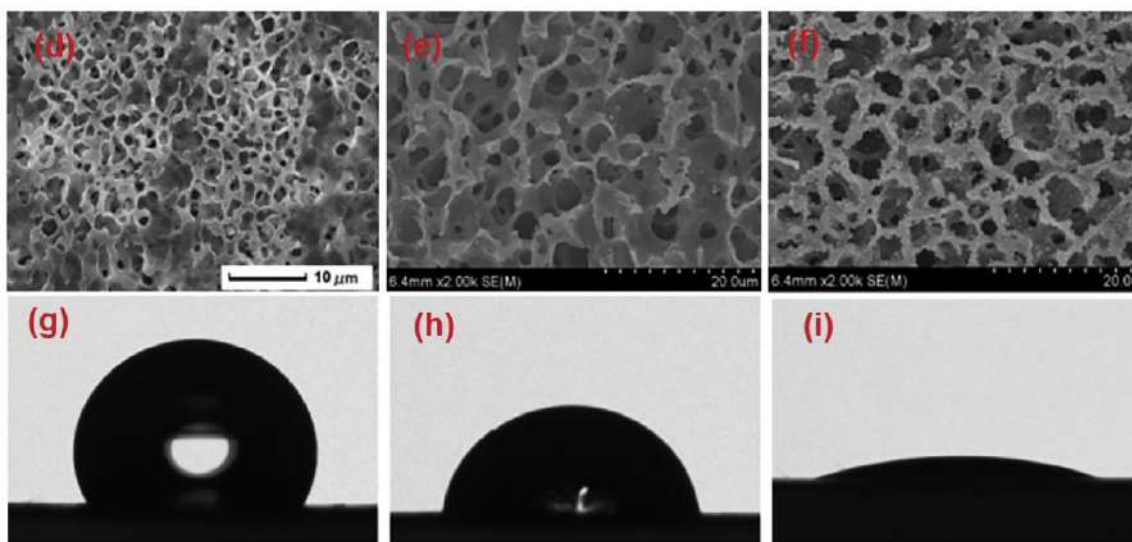


Figure 2.5. Water ($\theta > 150^\circ$) and oil ($\theta \approx 0^\circ$) contact angles on a PVDF@PDA@SiO₂ nanocomposite membrane, demonstrating the coexistence of superhydrophobic and superoleophilic states that enables efficient oil–water separation. In the original study, the PVDF base provides a chemically resistant, mechanically robust support; a polydopamine (PDA) interlayer improves adhesion and introduces functional groups; and the top SiO₂ nanoparticle coating generates hierarchical roughness, which, together with the low surface energy of the polymer, produces a Cassie–Baxter state for water (large θ , water droplets roll off) and a Wenzel-like, fully wetted state for oil ($\theta \approx 0^\circ$, rapid imbibition). This asymmetry in wetting behavior allows the membrane to selectively and rapidly pass oil while strongly rejecting water, directly illustrating the Young, Wenzel, and Cassie–Baxter concepts introduced in Section 2.3 of the manual, where surface chemistry and nano/micro-roughness are linked to the design of nanocomposite materials for gravity-driven oil–water separation. [Khodakarami, M. & Bagheri, M. Recent advances in synthesis and application of polymer nanocomposites for water and wastewater treatment. *Journal of Cleaner Production*, 2021, 296, 126404. Fig. 28g–i. doi:10.1016/j.jclepro.2021.126404]

Chapter 3. Nanophotocatalysis: Converting Solar Energy into Environmental Action

Photocatalysis represents one of the most promising "green" technologies for environmental remediation, utilizing semiconductor-based nanocomposites to drive the chemical degradation of persistent organic pollutants, pathogens, and heavy metals using light energy [35, 36]. This chapter explores the physical principles of charge carrier dynamics and energy band engineering that determine the efficiency and safety of these materials.

3.1. Charge Generation, Recombination, and Carrier Separation Efficiency

The fundamental operation of a nanophotocatalyst is based on the excitation of electrons from the valence band (VB) to the conduction band (CB) upon the absorption of a photon with energy equal to or greater than the material's bandgap (E_g). This process creates an electron-hole pair e^-/h^+ . The pair must reach the surface before recombining for photocatalysis to occur [35, 36].

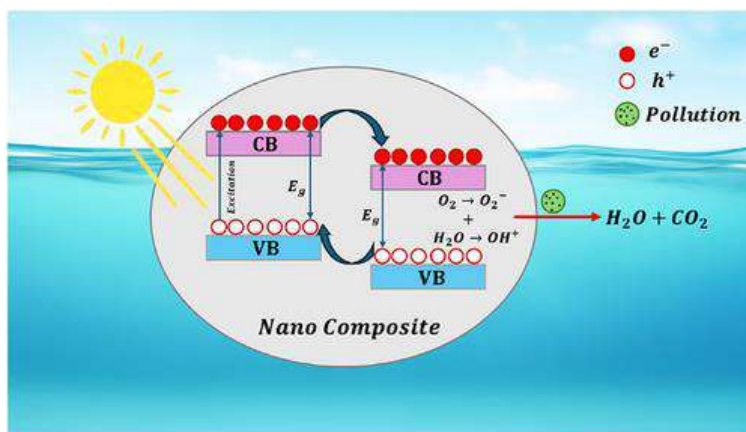


Figure 3.1. Mechanism of photocatalysis on semiconductor nanocomposites: incident photons with energy equal to or greater than the bandgap E_g are absorbed, promoting electrons from the valence band (VB) to the conduction band (CB) and generating electron-hole pairs (e^-/h^+). The photogenerated electrons then migrate to surface or interfacial sites, where they reduce dissolved O_2 to superoxide radicals ($\cdot O_2^-$) and, via further proton-coupled steps, to hydroxyl radicals ($\cdot OH$), while the photogenerated holes move toward oxidizing surface sites, where they directly oxidize pollutants or react with H_2O/OH^- to form $\cdot OH$. These reactive oxygen species (ROS) initiate a cascade of redox reactions that progressively break down organic contaminants into smaller intermediates and ultimately mineralize them to CO_2 , H_2O , and inorganic ions. In the context of this manual, the figure provides the unifying physical picture for Chapter 3: it connects the bandgap engineering and carrier separation strategies discussed in Section 3.1 (heterojunctions, Z-schemes, Schottky contacts) with the environmental function of nanophotocatalysts, namely using sunlight to drive ROS-mediated degradation of persistent pollutants in water and air. [Sharshir, S.W. et al. Recent advances in photocatalytic nanomaterials for environmental remediation and solar-driven water treatment systems. *Global Challenges*, 2025, 9(10), e00217. Fig. 8. doi:10.1002/gch2.202500217]

3.1.1. Bandgap Engineering: TiO_2 , ZnO , and WO_3

In physics, the E_g determines the minimum energy required to initiate photocatalysis [36].

- **Titanium Dioxide (TiO₂):** Anatase TiO₂ (E_g ≈ 3.2 eV) and Rutile (E_g ≈ 3.0 eV) are the benchmarks due to their high stability and low toxicity. However, their wide bandgap restricts activity mainly to the UV spectrum (λ < 388 nm), which is only ~5% of sunlight.
- **Zinc Oxide (ZnO):** Similar to TiO₂, ZnO has a bandgap of ~3.2–3.4 eV. While efficient, it suffers from photo-corrosion at extreme pH levels.
- **Tungsten Trioxide (WO₃):** With a narrower bandgap (E_g ≈ 2.4–2.8 eV), WO₃ is visible-light responsive, but its conduction band potential is often too low for direct oxygen reduction.

Physics Highlight | Quantum Efficiency Φ and Carrier Separation Efficiency η_{sep}

Quantum efficiency (quantum yield) — key figure of merit for comparing photocatalysts [36, 37]:

$$\Phi = (\text{number of product molecules formed per unit time}) / (\text{number of photons absorbed per unit time}) \quad [\text{dimensionless, } 0 < \Phi \leq 1]$$

Apparent quantum yield AQY uses incident (not absorbed) photon flux:

$$\text{AQY} = (\text{rate of pollutant degradation [mol/s]}) / (\text{incident photon flux [mol/s]})$$

Typical values: pure TiO₂ → AQY ≈ 1–3% (UV);

TiO₂/Ag/g-C₃N₄ heterostructure → AQY ≈ 8–15% (visible light). [37]

Carrier separation efficiency η_{sep} [37]:

$$\eta_{\text{sep}} = \tau_r / (\tau_r + \tau_d) = 1 / (1 + D / (\tau_r \cdot r^2))$$

where:

τ_r — recombination time [s] (bulk TiO₂: ~10⁻¹⁰–10⁻⁹ s;

TiO₂/Ti₃C₂ Schottky heterostructure: ~10⁻⁷ s → 100× longer);

τ_d — diffusion time to surface = r²/D [s];

D — carrier diffusion coefficient [m²/s] (e⁻ in TiO₂: D ≈ 10⁻¹² m²/s);

r — nanoparticle radius [m].

Physical insight: reducing r from 100 nm to 5 nm decreases τ_d by a factor of 400, raising η_{sep} dramatically — the fundamental reason why nanoparticles outperform microparticle photocatalysts. [37]

3.1.2. Physics of Heterojunctions and Z-Schemes

To overcome the "recombination paradox"—where e⁻/h⁺ pairs recombine within nanoseconds before they can react—physicists design heterojunctions.

- **Schottky Barriers:** Interfaces between semiconductors and conductive 2D materials like MXenes (e.g., Ti₃C₂) create a built-in electric field. This barrier traps electrons on the MXene surface, effectively separating them from the holes in the semiconductor.
- **Z-Scheme Systems:** These mimic natural photosynthesis by using two semiconductors with staggered band structures. Electrons from the CB of one material recombine with holes from the VB of the other, preserving the strongest oxidative and reductive potentials in the system.

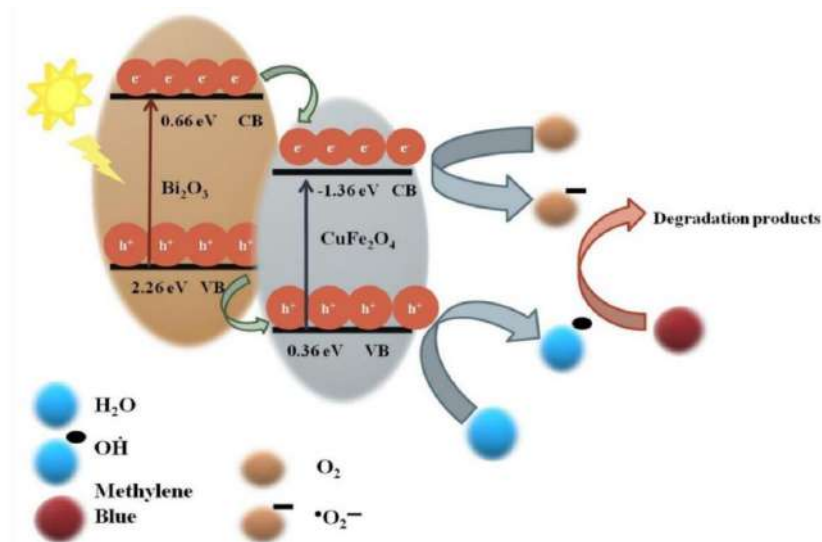


Figure 3.2. Schematic mechanism of photocatalytic degradation of organic pollutants using a $\text{CuFe}_2\text{O}_4/\text{Bi}_2\text{O}_3$ magnetic nanocomposite: under visible-light irradiation, Bi_2O_3 (n-type) and CuFe_2O_4 (p-type) form a p–n heterojunction that facilitates spatial separation of photogenerated charge carriers. Electrons excited in the conduction band of Bi_2O_3 (or transferred from the CuFe_2O_4 side, depending on band alignment) migrate to surface active sites, where they reduce dissolved O_2 to $\cdot\text{O}_2^-$ and, through subsequent steps, to $\cdot\text{OH}$, while photogenerated holes remaining in the complementary valence band oxidize surface-adsorbed $\text{H}_2\text{O}/\text{OH}^-$ to $\cdot\text{OH}$ and can also directly oxidize organic molecules. These reactive oxygen species (ROS) cooperatively attack and decompose organic pollutants into smaller intermediates and ultimately mineralize them to CO_2 , H_2O , and inorganic ions, while the ferrite core imparts magnetic recoverability to the catalyst, enabling easy post-treatment separation and reuse. In the context of this manual, the figure illustrates how heterojunction engineering (Section 3.1) and magnetic nanocomposite design (Section 3.2) are combined in practice to enhance charge separation, extend light absorption, and simplify catalyst recovery in real photocatalytic water-treatment processes. [Sharshir, S.W. et al. Recent advances in photocatalytic nanomaterials for environmental remediation and solar-driven water treatment systems. *Global Challenges*, 2025, 9(10), e00217. Fig. 11b. doi:10.1002/gch2.202500217.]

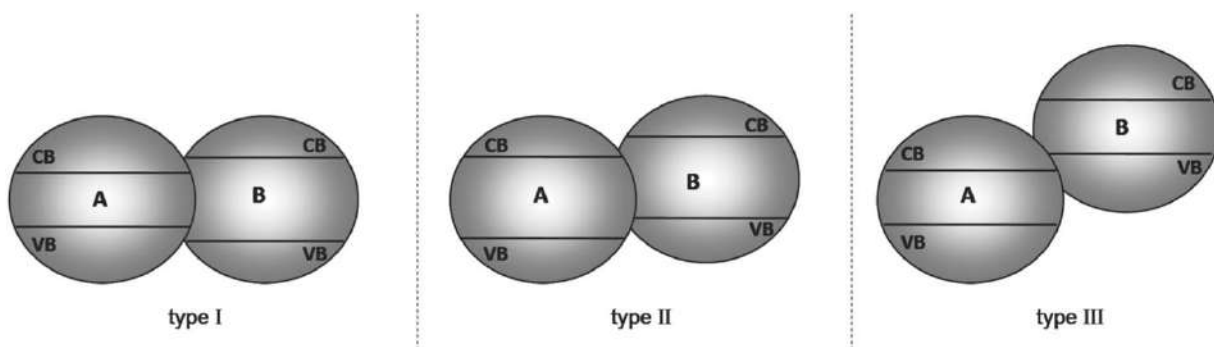


Figure 3.3 Band structure diagrams illustrating charge carrier transfer mechanisms in semiconductor heterojunction photocatalysts: (a) Type I (straddling gap) — the conduction band (CB) and valence band (VB) of semiconductor B straddle those of semiconductor A; both photogenerated electrons (e^-) and holes (h^+) accumulate in the narrower-bandgap semiconductor, so recombination remains high and photocatalytic activity is not significantly improved relative to single-component materials. (b) Type II (staggered gap) — the CB of B lies at a more negative potential than that of A, while the VB of A is more positive than that of B; upon illumination, electrons preferentially transfer to CB(A) and holes to VB(B), realizing spatial charge separation and strongly suppressing recombination, which explains why this architecture underpins many of the nanocomposite photocatalysts discussed in Section 3.1 of this manual.

manual. (c) Z-scheme — inspired by natural photosynthesis, where electrons in CB(B) recombine with holes in VB(A) via a solid, redox, or direct-contact mediator, leaving the most reducing electrons in CB(A) and the most oxidizing holes in VB(B); this configuration simultaneously maintains strong redox power and spatial charge separation, making it particularly suitable for thermodynamically demanding processes such as complete pollutant mineralization, overall water splitting, and H₂O₂ generation considered in Chapter 3. [Schumacher, L. & Marschall, R. Band alignment and charge transfer in semiconductor heterojunction photocatalysts. *Top. Curr. Chem.*, 2022, 380, 53. Figs. 3, 6. doi:10.1007/s41061-022-00406-5]

3.2. Absorption Spectrum Control: Doping and Surface Plasmon Resonance

Broadening the response of nanocomposites from the UV into the visible and near-infrared (NIR) regions is essential for practical solar applications.

3.2.1. Doping and Mid-Gap States

Doping involves introducing impurities into the crystal lattice to create localized energy levels within the forbidden zone.

- **Non-Metal Doping:** Doping with Nitrogen (N), Carbon (C), or Sulfur (S) can narrow the effective bandgap or introduce states above the VB, enabling visible light absorption without drastically shifting the CB potential. (N-doped TiO₂ absorbs up to ~520 nm vs 388 nm for undoped [38])
- **Metal Doping:** Transition metals (e.g., Fe, Cr) introduce d-orbitals that act as electron or hole traps, though excessive doping can create recombination centers that reduce quantum yield.

3.2.2. Surface Plasmon Resonance (SPR)

The inclusion of noble metal nanoparticles (Ag, Au) into the composite allows for Plasmon-enhanced photocatalysis [39].

- **Physical Mechanism:** When light strikes the metal nanoparticles, it induces collective oscillations of conduction electrons (plasmons). This generates a strong local electromagnetic field that enhances light absorption in the adjacent semiconductor and can inject "hot electrons" into its conduction band, significantly increasing reaction rates in the visible spectrum.

Physics Highlight | Drude Dielectric Function and LSPR Resonance Condition

Drude dielectric function of a metal nanoparticle [39]:

$$\epsilon_m(\omega) = \epsilon_\infty - \omega_p^2 / (\omega^2 + i\gamma\omega)$$

where:

$\epsilon_m(\omega)$ — complex dielectric function of the metal at angular frequency ω ;

ϵ_∞ — high-frequency dielectric constant (~1 for free-electron metals);

ω_p — bulk plasma frequency [rad/s];

Au: $\omega_p \approx 1.37 \times 10^{16}$ rad/s; Ag: $\omega_p \approx 1.38 \times 10^{16}$ rad/s;

ω — angular frequency of incident light [rad/s];

γ — electron damping rate [rad/s] (related to mean free path);

i — imaginary unit.

Fröhlich condition for Localized Surface Plasmon Resonance (LSPR) in a spherical nanoparticle in a dielectric matrix [39]:

$$\text{Re}[\epsilon_m(\omega_{\text{res}})] = -2 \cdot \epsilon_d$$

ω_{res} — LSPR angular frequency [rad/s];

ϵ_d — real part of the dielectric permittivity of the surrounding matrix.

Practical consequence:

Au in TiO_2 ($\epsilon_d \approx 5.5$) $\rightarrow$ LSPR peak at $\lambda \approx 520\text{--}550$ nm (green).

Ag in TiO_2 ($\epsilon_d \approx 5.5$) $\rightarrow$ LSPR peak at $\lambda \approx 400\text{--}450$ nm (violet–blue).

$\rightarrow$ Noble metal addition extends effective photocatalytic activity into visible range. [39]

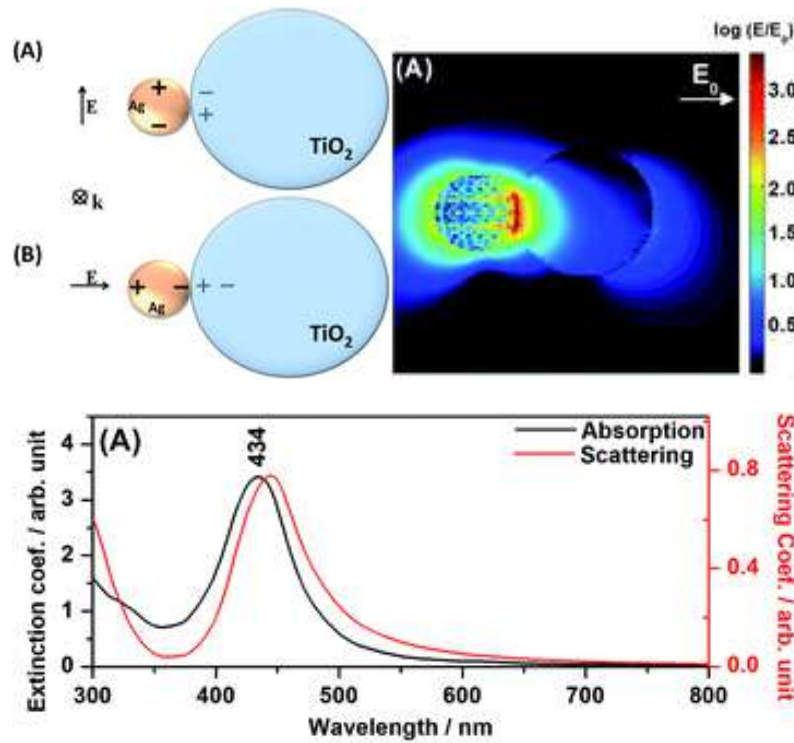


Figure 3.4 Localized surface plasmon resonance (LSPR) in an Ag/ TiO_2 nanocomposite photocatalyst: (a) schematic of the LSPR mechanism — incident visible light excites a collective oscillation of conduction electrons in Ag nanoparticles (dipole mode), and when the LSPR energy ($\hbar\omega_{\text{res}} \approx 2.8$ eV, $\lambda \approx 435\text{--}464$ nm) is resonant with the TiO_2 bandgap ($E_g \approx 3.2$ eV, anatase), the resulting image charge in TiO_2 strongly enhances the local electric field at the Ag– TiO_2 interface and increases the probability of e^-/h^+ pair generation. (b) DDA-simulated extinction spectra (absorption + scattering) of the TiO_2/Ag composite show an LSPR maximum at 434 nm that overlaps with the TiO_2 band edge, redshifted relative to isolated Ag nanoparticles in water (388 nm) due to the higher dielectric constant of TiO_2 , thus shifting the resonance into the visible range and enabling visible-light photocatalysis. (c) The corresponding DDA near-field enhancement map $|E/E_0|^2$ at 434 nm reveals an electric field amplification of about three orders of magnitude at the metal–semiconductor interface with significant penetration into TiO_2 , which explains the LSPR-enhanced photocatalytic performance and serves, within this manual, as a model example of how plasmonic nanostructures (Section 3.3) extend light harvesting and reinforce the charge-generation strategies introduced in

Section 3.1. [Lemos de Souza, M. et al. Electromagnetic mechanism of plasmon-enhanced photocatalysis in Ag/TiO₂ nanocomposites revealed by DDA simulations. RSC Advances, 2018, 8, 28753. Figs. 6a, 7a, Scheme 2. doi:10.1039/C8RA03919D.]

3.3. Mineralization of Organic Pollutants

The ultimate goal of photocatalysis is the complete mineralization of toxic organic molecules into harmless products like CO₂, H₂O, and inorganic ions.

3.3.1. Formation of Reactive Oxygen Species (ROS)

The charge carriers that reach the surface participate in redox reactions with water and oxygen [35, 36]:

1. Oxidation: $h^+ + \text{H}_2\text{O} \rightarrow \text{OH}^\bullet$ (hydroxyl radical; $E^\circ = +2.80 \text{ V}$).
2. Reduction: $e^- + \text{O}_2 \rightarrow \text{O}_2^{\bullet-}$ (superoxide radical anion; $E^\circ = -0.33 \text{ V}$).

These ROS are non-selective and possess extremely high oxidation potentials, enabling them to break down complex aromatic rings in dyes, antibiotics, and pesticides [35].

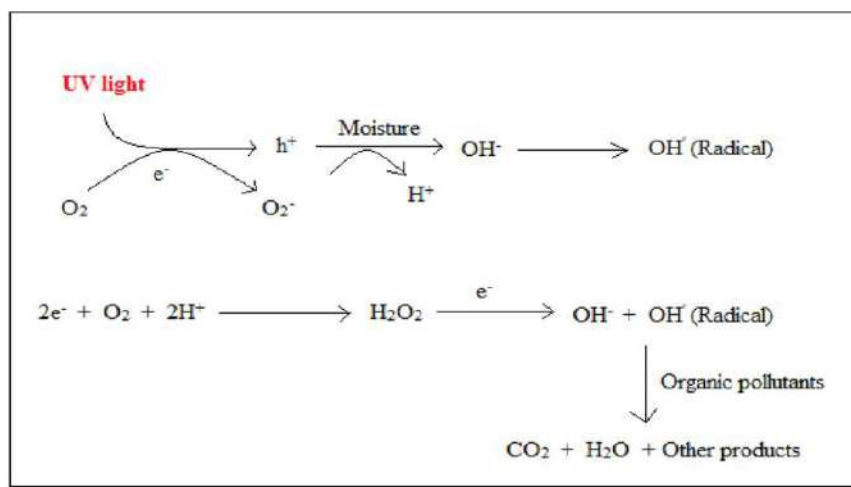


Figure 3.5. Pathway of organic dye degradation and reactive oxygen species (ROS) formation under light irradiation in a nanocomposite photocatalytic system: incident photons with suitable energy excite electrons from the valence band to the conduction band of the semiconductor component of the nanocomposite, generating electron–hole pairs that migrate to the surface and participate in redox reactions with adsorbed species. Conduction-band electrons reduce dissolved O₂ to superoxide radicals ($\cdot\text{O}_2^-$), which via subsequent protonation and disproportionation steps yield hydrogen peroxide (H₂O₂) and hydroxyl radicals ($\cdot\text{OH}$), while valence-band holes oxidize surface-bound dye molecules directly or react with H₂O/OH⁻ to form additional $\cdot\text{OH}$; these ROS attack the chromophoric structure of the dye, leading to decolorization, fragmentation into smaller intermediates, and eventual mineralization to CO₂, H₂O, and inorganic ions. In the context of this manual, the figure links the general photocatalytic mechanism from Chapter 3 with practical dye-removal applications, illustrating how nanocomposite design (band-gap tuning, heterojunction formation, and co-catalyst integration) is used to enhance charge separation, maximize ROS generation, and thereby improve the efficiency and sustainability of photocatalytic wastewater treatment processes discussed in Sections 3.2–3.3. [Joshi, N.C. & Gururani, P. Photocatalytic degradation of organic dyes using nanocomposite materials: mechanisms and sustainability aspects. Current Research in Green and Sustainable Chemistry, 2022, 5, 100248, Fig. 5. doi:10.1016/j.crgsc.2022.100248]

Comparative Table: Key Photocatalytic Nanocomposite Systems

Material	E _g (eV)	Light range	Target pollutant	AQY (%)	Reference
TiO ₂ anatase	3.2	UV	Dyes, micropollutants	1–3	[36]
ZnO	3.37	UV	Dyes, heavy metals	2–5	[36]
WO ₃	2.6	Visible	Persistent organics	3–8	[36]
TiO ₂ /Ag (LSPR)	2.9*	UV-Vis	Dyes, bacteria	8–12	[39]
TiO ₂ /Ti ₃ C ₂ MXene	3.0*	UV-Vis	Pharmaceuticals	10–15	[22]
g-C ₃ N ₄ /TiO ₂ Z-scheme	2.7*	Visible	Antibiotics, dyes	12–18	[35]
CuFe ₂ O ₄ /Bi ₂ O ₃	2.2*	Vis-NIR	Dyes, micropollutants	7–11	[35]

* Effective optical bandgap shifted by doping, heterostructure, or LSPR effect. Sources: [22, 35, 36, 39].

Chapter 4. Physical Aspects of Nanotoxicology and Safety

Nanotoxicology evaluates the hazards of engineered nanomaterials (ENMs) by analyzing their physicochemical and biological interactions. For physicists, the risk profile of a nanocomposite is not just a function of its chemical toxicity but is intrinsically linked to its physical parameters: size, shape, surface energy, and the mechanics of its interaction with biological barriers [41, 42].

4.1. Mechanical and Chemical Destruction of Cells

The biocidal efficiency of nanocomposites, while useful for water disinfection, poses a direct risk to non-target microorganisms and human cells. The primary physical pathways of destruction include mechanical piercing and the induction of biochemical imbalances.

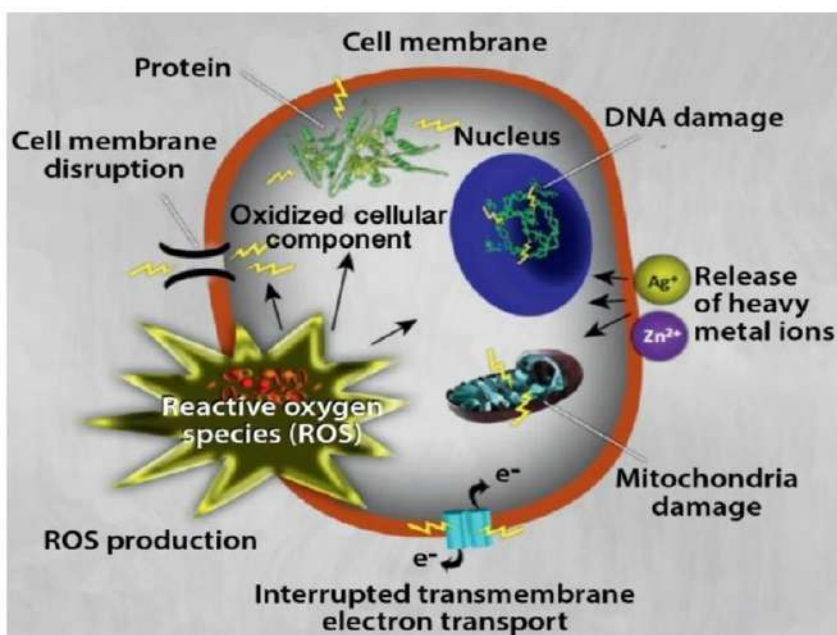


Figure 4.1. Mechanisms of nanoparticle toxicity against bacteria: (a) physical membrane disruption by 1D (nanorods, nanotubes) and 2D (nanosheets) nanostructures acting as “nano-darts” that pierce, stretch, or locally deform the cell envelope, increasing permeability and causing leakage of cytoplasmic contents; (b) generation of reactive oxygen species (ROS) at the nanoparticle surface or via photo-/redox reactions (e.g., $\cdot\text{OH}$, $\cdot\text{O}_2^-$, H_2O_2), which oxidatively damage membrane lipids, proteins, and nucleic acids, ultimately compromising membrane integrity and vital cellular functions; (c) release of toxic metal ions (such as Ag^+ , Cu^{2+} , Zn^{2+}) from metal oxide or metal-containing nanocomposites, with ions binding to thiol groups in proteins, disrupting respiratory chains, and interfering with DNA replication. In the context of this manual, the figure serves as a conceptual bridge between the structure–property relationships of nanocomposites discussed in Section 4 and their practical antimicrobial performance in water treatment systems, highlighting how morphology, composition, ROS generation, and ion release collectively determine efficacy and selectivity. [Shirsat, S.D. et al. *Metal Oxide Nanocomposites in Water and Wastewater Treatment*, Elsevier, 2021, Fig. 14.9]

4.1.1. Physical Membrane Damage by "Nano-Darts"

One-dimensional (1D) nanostructures like carbon nanotubes (CNTs) and two-dimensional (2D) sheets like graphene act as physical "nano-darts".

- **Needle-like Penetration:** Microorganisms lose viability upon contact with CNTs because the nanometer-sized fibers easily penetrate through bacterial cell walls. This physical impingement leads to cell lysis and the subsequent release of intracellular contents [41, 42].
- **Surface Roughness:** Rough MXene surfaces have also been reported to cause the mechanical destruction of microbial membranes, effectively decreasing bacterial growth through physical disruption [43].

4.1.2. Oxidative Stress and DNA Damage

Oxidative Stress and DNA Damage: beyond mechanical impact, the unique electronic properties of nanomaterials drive chemical toxicity.

- **Reactive Oxygen Species (ROS):** Many metal oxide nanoparticles (TiO_2 , ZnO , CuO) generate ROS—such as hydroxyl radicals and superoxide anions—upon photosensitization. These species cause oxidative stress, leading to lipid peroxidation and the destruction of cellular proteins[41].
- **Genotoxicity:** Nanoparticles can penetrate the nucleus or interact with phosphorus moieties in DNA, disrupting replication. For example, commercial pesticides like deltamethrin show significantly lower DNA damage when adsorbed onto iron-oxide nanocomposites compared to their free form, illustrating the potential of composites to "buffer" toxic chemical signals[42].

4.2. Physics of Leaching, DLVO Theory, and Migration in Soil

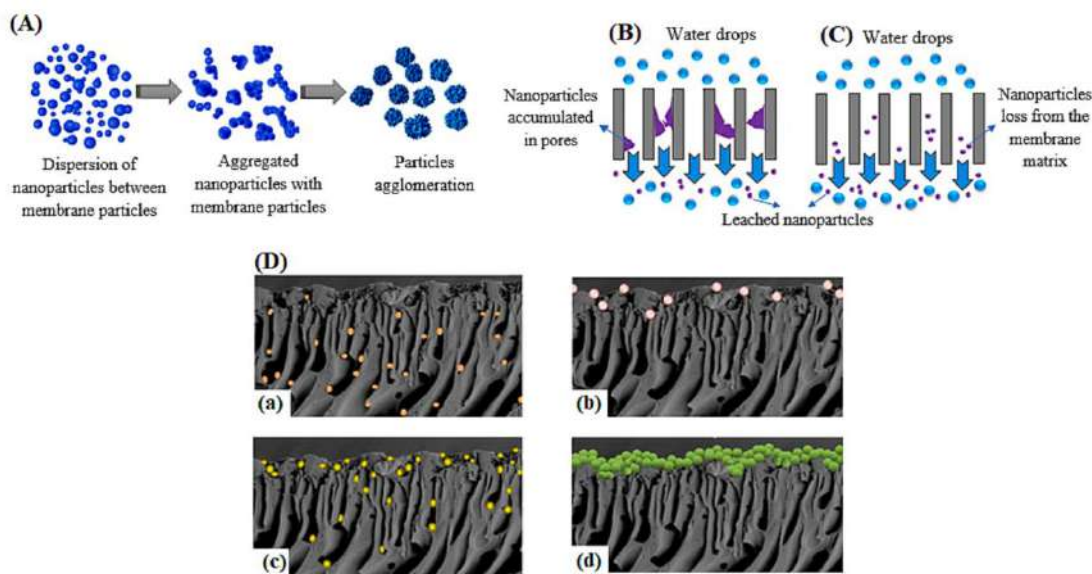


Figure 4.2. Nanoparticle leaching through membrane pores and agglomeration within a composite matrix: schematic illustration of how embedded antimicrobial or catalytic nanoparticles can gradually escape from the selective layer into the permeate side when their size approaches or falls below the effective pore diameter, or when defects, microcracks, and weak polymer–filler interfacial adhesion create additional leakage pathways. In parallel, nanoparticles that are insufficiently stabilized tend to agglomerate inside the polymer matrix or near pore walls, which reduces the available active surface area, blocks transport pathways, and leads to a loss of functional performance over time. In the context of this manual, the figure emphasizes that designing nanocomposite membranes for water treatment (Sections 4.2–4.3) requires not only maximizing initial activity (antimicrobial or catalytic) but also engineering strong

nanoparticle–matrix interactions, appropriate particle size, and pore structure to minimize leaching and aggregation over realistic operating lifetimes. [Omar, N.M.A. et al. Long-term stability and leaching behavior of antimicrobial nanoparticles in polymeric water treatment membranes. J. Water Process Engineering, 2024, 59, 104952, Fig. 4A,B. doi:10.1016/j.jwpe.2024.104952]

A critical safety concern is the release of nanoparticles from composite matrices, causing secondary pollution in soil and groundwater [44, 45]. Stability of fixation depends on the quality of interfacial bonding: improper sintering leaves nanoparticles loosely held; UV radiation and mechanical stress can cause matrix microcracks [44].

4.2.1. Stability of Fixation in Matrices

The retention of nanofillers within a matrix (polymer or ceramic) is governed by the strength of interfacial bonding.

- **Sintering and Bonding:** In ceramic membranes, improper control of sintering temperatures leads to incomplete bonding, rendering nanoparticles loosely held and susceptible to leaching into treated water.
- **Matrix Degradation:** Exposure to UV radiation, mechanical stress (stretching or pressure), and chemical erosion can physically damage the matrix, creating microcracks that facilitate nanoparticle release.
- **Release Rates:** In nano-enabled textiles, silver nanoparticles (nAg) can leach at rates ranging from 0.32 to 38.5 mg/L during standard washing cycles.

4.2.2. Size and Charge Effects on Diffusion

Once released, the migration of nanomaterials in soil and water is determined by their physical state.

- **Particle Size:** Smaller particles have higher mobility in porous soil media but are also more likely to pass through the sieving layers of filtration membranes.
- **Surface Charge and pH:** The mobility of nanoparticles in the rhizosphere is influenced by the soil's pH and ionic strength, which affect the zeta potential and the tendency of particles to either aggregate (settle) or remain suspended (migrate).
- **Adsorption-Desorption Dynamics:** Migration between soil and groundwater is often irreversible if the nanoparticles form strong chemical or electrochemical bonds with soil organic matter.

Physics Highlight | DLVO Theory: Colloidal Stability of Nanoparticles in Soil

The DLVO (Derjaguin–Landau–Verwey–Overbeek) theory describes the total interaction potential V_T between two nanoparticles in aqueous medium [45]:

$$V_T(h) = V_{EDL}(h) + V_{vdW}(h)$$

where:

V_T — total interaction energy [J];

h — separation distance between particles [m];
 V_{EDL} — electrical double layer (EDL) repulsion energy [J];
 V_{vdW} — van der Waals attraction energy [J].

For two identical spherical particles of radius r [45]:

$$V_{EDL}(h) = 64\pi r n_0 k_B T \cdot \kappa^{-1} \cdot \gamma^2 \cdot \exp(-\kappa h)$$

$$\gamma = \tanh(z \cdot e \cdot \psi_0 / 4k_B \cdot T)$$

n_0 — bulk electrolyte concentration [ions/m³];
 κ^{-1} — Debye screening length [m]: $\kappa^{-1} = \sqrt{(\epsilon \cdot \epsilon_0 \cdot k_B \cdot T) / (2n_0 \cdot z^2 \cdot e^2)}$;
 ψ_0 — surface potential [V] (related to zeta potential ζ in experiments);
 z — ion valence; e — elementary charge (1.6×10^{-19} C).

$$V_{vdW}(h) = -A_H \cdot r / (12h)$$

A_H — Hamaker constant [J] (for metal oxides in water: $A_H \sim 10^{-20}$ – 10^{-19} J).

Key consequences for environmental risk assessment:

1. High ionic strength (concentrated soil solution): κ increases $\rightarrow \kappa^{-1}$ decreases
 $\rightarrow V_{EDL}$ is screened $\rightarrow$ energy barrier disappears $\rightarrow$ particles aggregate and settle.
2. Low ionic strength (dilute groundwater): energy barrier $V_{max} = V_{EDL} + V_{vdW}$
 remains high $\rightarrow$ particles remain dispersed and mobile $\rightarrow$ long-range migration.
3. pH affects ψ_0 : at pH = PZC (point of zero charge) the barrier collapses
 regardless of ionic strength $\rightarrow$ maximum aggregation. [45]

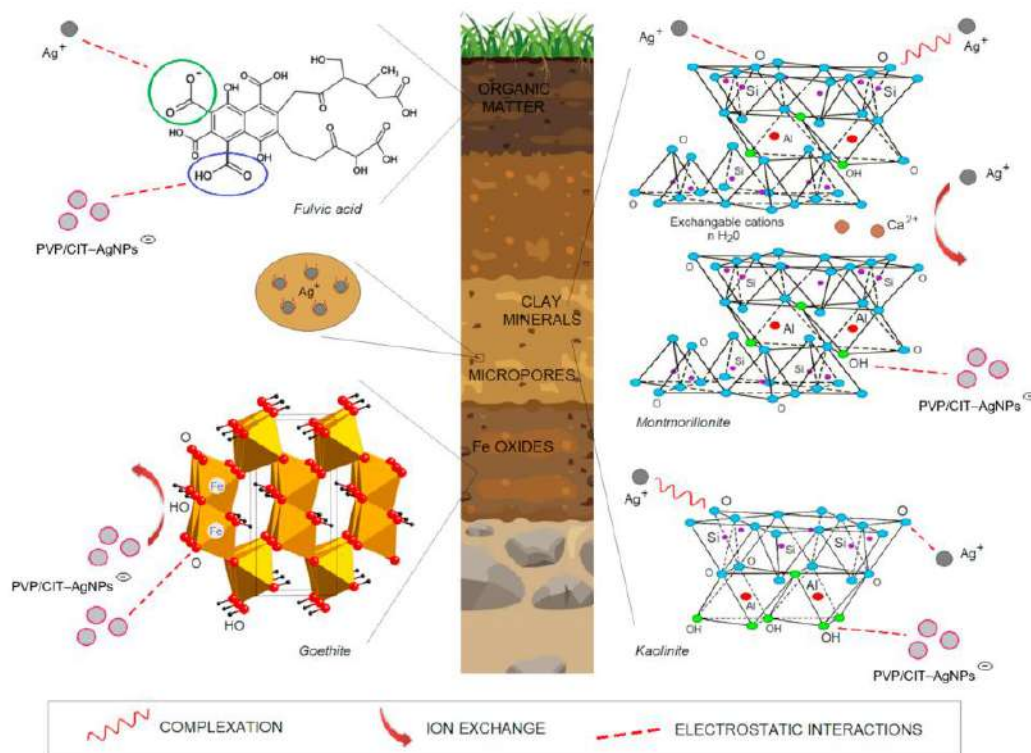


Figure 4.3 Interactions of negatively charged PVP/citrate-coated Ag nanoparticles (PVP/CIT–AgNPs[−]) with the main soil components: complexation with fulvic acid functional groups (–COOH, –OH); ion exchange and electrostatic repulsion at clay mineral surfaces (montmorillonite, kaolinite); and electrostatic repulsion from Fe-oxide (goethite) surface hydroxyl groups, which collectively control nanoparticle retention versus mobility in the soil pore network. Ag⁺ ions released from dissolving AgNPs compete for the same binding sites via ion exchange and complexation, so both particulate and ionic silver species are governed by soil organic matter, clay mineralogy, and pH-dependent surface charge. In the context of this manual, the figure illustrates how the colloidal stability and transport of engineered nanocomposites in subsurface environments (Section 4.4) depend not only on particle coating and charge but also on specific interactions with natural organic matter and mineral surfaces, which in turn determine the balance between immobilization, long-range migration, and potential ecotoxicological impact. [Kyziol-Komosinska, J. et al. Mobility and retention of polyvinylpyrrolidone/citrate-coated silver nanoparticles in model soil systems. *Molecules*, 2024, 29, 5531, Fig. 3. doi:10.3390/molecules29235531]

4.3. Aerosol Physics: Stokes–Einstein Diffusion and ICRP Deposition Model

Inhalation is the most significant exposure route for individuals working in the production of nanocomposites.

4.3.1. Physics of Aerosols and Inhalation

- **Respirable Fraction:** Nanoparticles (<100 nm) belong to the respirable fraction and can penetrate to the alveolar region of the lungs [42, 46].
- **Deposition Probability:** Smaller particles (1 nm) have a 90% probability of depositing in the nasopharyngeal region, while 5 nm particles deposit equally (30%) across the nasopharyngeal, tracheobronchial, and alveolar regions [42].
- **Generation during Processing:** Airborne nanoparticles are frequently emitted during weighing, molding, and sonication (aqueous dispersion) of carbon-based fillers [46].

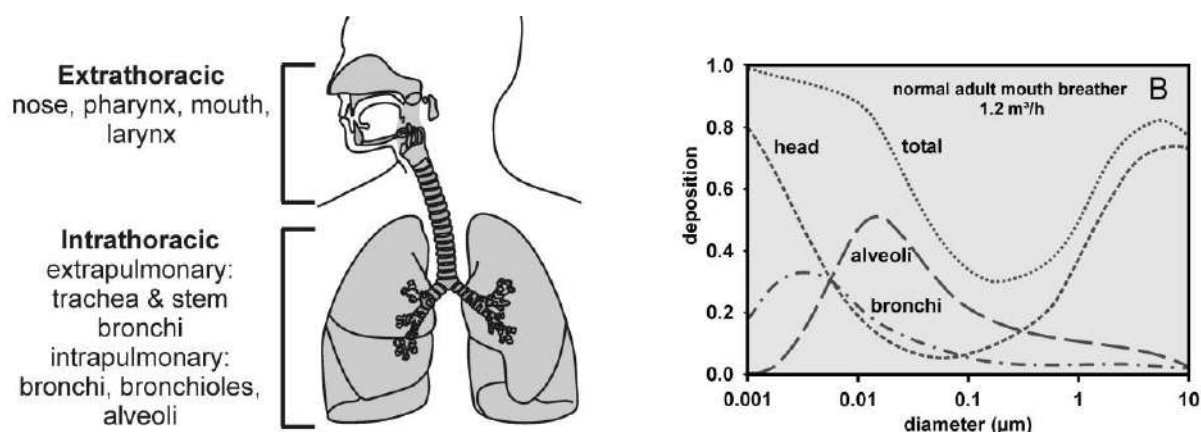


Figure 4.4. Regional deposition fractions of inhaled particles in the human respiratory tract as a function of thermodynamic (< 0.5 μm) or aerodynamic (> 0.5 μm) diameter, based on the ICRP Human Respiratory Tract Model (HRTM) for a healthy adult at light-workload breathing: three anatomical regions are shown — extrathoracic

(nasopharyngeal; blue), bronchiolar/tracheobronchial (conducting airways; green), and alveolar (peripheral lung; red). The curves highlight three key physical regimes: (i) for particles < 100 nm (nanoparticle range), Brownian diffusion dominates, so total deposition rises sharply as diameter decreases and can approach ~90% at $d \approx 1$ nm; (ii) around $d \approx 0.5$ μm , overall deposition exhibits a minimum of roughly 20%, because neither diffusion nor inertial impaction/sedimentation are efficient; (iii) for particles > 1 μm , inertial impaction and gravitational settling become dominant, leading to increased deposition in the extrathoracic and tracheobronchial regions. In the context of this manual, the figure provides the physiological basis for the occupational safety recommendations in Section 4.3.3, explaining why engineered nanocomposite dusts in the 10–100 nm range are of particular concern and why high-efficiency respiratory protection (e.g., FFP3) and engineering controls are required to limit deep alveolar exposure. [Geiser, M. & Kreyling, W.G. Deposition and biokinetics of inhaled nanoparticles in the human respiratory tract. Part. Fibre Toxicol., 2010, 7, 2, Fig. 6. doi:10.1186/1743-8977-7-2]

Physics Highlight | Stokes–Einstein Diffusion Coefficient and Stokes Number

Diffusion coefficient of a spherical nanoparticle in air (Stokes–Einstein) [46]:

$$D = (k_B \cdot T \cdot C_c) / (3\pi \cdot \eta_{\text{air}} \cdot d_p)$$

where:

- D — diffusion coefficient of the nanoparticle [m^2/s];
- k_B — Boltzmann constant (1.38×10^{-23} J/K);
- T — temperature [K] (at $37^\circ\text{C} = 310$ K in the lungs);
- C_c — Cunningham slip correction factor (for $d_p < 100$ nm, $C_c \gg 1$;
for $d_p = 10$ nm in air at 37°C : $C_c \approx 22$);
- η_{air} — dynamic viscosity of air ($\eta_{\text{air}} \approx 1.9 \times 10^{-5}$ Pa·s at 37°C);
- d_p — aerodynamic particle diameter [m].

Numerical example:

$d_p = 10$ nm: $D \approx (1.38 \times 10^{-23} \times 310 \times 22) / (3\pi \times 1.9 \times 10^{-5} \times 10^{-8})$
 $\approx 5.2 \times 10^{-8}$ m^2/s — 1000× larger than for 1 μm particles.
 → Nanoparticles diffuse rapidly to airway walls, dramatically increasing alveolar deposition probability. [46]

Stokes number — governs inertial impaction (deposition at bends in airways) [46]:

$$\text{Stk} = (\rho_p \cdot d_p^2 \cdot U_o \cdot C_c) / (18 \cdot \eta_{\text{air}} \cdot d_{\text{aw}})$$

- ρ_p — particle density [kg/m^3] (TiO_2 : 4200 kg/m^3 ; carbon: 2260 kg/m^3);
 - U_o — flow velocity in the airway [m/s];
 - d_{aw} — airway diameter [m].
- For $d_p < 100$ nm: $\text{Stk} \ll 1 \rightarrow$ inertial impaction negligible;
 diffusion dominates $\rightarrow$ high alveolar deposition. [46]

4.3.2. Penetration of Biological Barriers

Once inhaled or absorbed, nanoparticles navigate biological systems through physical transport mechanisms:

- **Olfactory and Blood-Brain Barriers:** Inhaled ENMs can enter the central nervous system directly via the olfactory nerves, bypassing traditional barriers.
- **Dermal Penetration:** While healthy skin restricts penetration, hair follicles can act as depositories. Studies on quantum dots (QDs) show they can reach the dermis or epidermis within 24 hours.
- **Circulatory System Transfer:** Fine particles deposited in the alveoli can diffuse into the bloodstream, eventually accumulating in the liver, kidney, or bone marrow [42].

4.3.3. Exposure Control: Engineering, Administrative, and Personal Protective Measures

Given the demonstrated ability of nanoparticles to penetrate deep into the alveolar region and cross biological barriers, occupational exposure control is a multi-level engineering challenge. The hierarchy of controls proceeds from elimination of the hazard at the source to last-resort personal protection [42, 46].

Engineering Controls at the Source: The most effective strategy is to prevent nanoparticle release into the working environment before it occurs:

- **Local exhaust ventilation (LEV):** Fume hoods and enclosed gloveboxes equipped with HEPA filters (High-Efficiency Particulate Air, retention efficiency >99.97% for particles $\geq 0.3 \mu\text{m}$) are placed directly at the point of nanoparticle generation — weighing, mixing, sonication — to capture aerosols before they disperse into the room air.
- **Wet processes:** Performing synthesis and handling steps in aqueous suspension rather than in dry powder form dramatically reduces aerosol generation. The surface tension of the liquid binds nanoparticles into droplets too large and heavy to remain airborne for long.
- **Encapsulation within robust matrices:** Embedding nanoparticles permanently into a polymer, ceramic, or silica matrix prevents their release throughout the entire use phase of the product. For example, Fe_3O_4 nanoparticles cross-linked within a carboxymethyl cellulose hydrogel matrix show leaching rates as low as 0.005% after one year of use. This is simultaneously a Safe-by-Design measure (see Section 5.3) and an exposure control strategy.

Administrative Controls: Administrative measures reduce exposure through work organization rather than physical barriers:

- **Restricted access zones:** Areas where dry nanopowders are handled are designated as controlled zones with restricted entry, reducing the number of workers exposed.

- **Standard Operating Procedures (SOPs):** Written protocols specify the minimum quantity of nanomaterial to be handled, mandatory wet cleaning (never dry sweeping or compressed-air blowing), and waste disposal in sealed containers to prevent secondary aerosolization.

Personal Protective Equipment (PPE): PPE is the last line of defence, used in combination with — not instead of — engineering controls:

- **Respiratory protection:** FFP3 half-masks (Filtering Facepiece, Protection Class 3, European standard EN 149) retain $\geq 99\%$ of airborne particles at $0.3\ \mu\text{m}$ — the most penetrating particle size for fibrous filters — under tested flow conditions. This size coincides with the minimum of the filtration efficiency curve, where neither inertial impaction nor diffusion is dominant. For nanoparticles smaller than $0.1\ \mu\text{m}$, diffusion actually increases filtration efficiency above the FFP3 minimum, providing additional protection.
- **Protective clothing and gloves:** Impermeable nitrile gloves and disposable coveralls prevent dermal uptake. Note that standard latex gloves offer inadequate protection against nanoparticle penetration through pin-holes and material defects.
- **Eye protection:** Sealed safety goggles prevent nanoparticle deposition on the conjunctiva, which — like the nasal mucosa — can serve as an entry point into the bloodstream.

Chapter 5. Sustainable Design and Life Cycle Assessment

The integration of nanocomposites into environmental engineering must be evaluated through the lens of sustainability: energy balances, material flows, and stability kinetics define the 'greenness' of a technology [47, 48].

5.1. Green Synthesis: Physico-chemical Advantages

Green synthesis, often termed "biogenic synthesis," utilizes biological entities—plants, bacteria, fungi, and algae—as "bio-nano factories" to produce nanoparticles. This approach offers a bottom-up alternative to conventional physical and chemical methods, which frequently rely on toxic reducing agents like sodium borohydride or hydrazine [47, 49].

- **Mechanisms of Bioreduction:** Biomolecules such as polyphenols, flavonoids, and proteins present in plant extracts possess ideal redox potentials that allow for the efficient reduction of metal precursors into their corresponding metallic states. For example, phenolic groups (Ph-OH) in tannins can reduce iron salts to iron oxide (Fe_3O_4) nanoparticles while simultaneously acting as stabilizing agents [49].
- **Stabilization and Capping:** A significant physical advantage of green synthesis is the in-situ "capping" of nanoparticles. Natural polymers and enzymes secrete metabolic intermediates that coat the particle surface, preventing aggregation (a common problem in classical physics of colloids) without the need for expensive synthetic surfactants [47].
- **Low-Energy Requirements:** Unlike gas-phase synthesis or plasma processes, biogenic routes typically operate at room temperature and atmospheric pressure, significantly reducing the primary energy input required during the manufacturing stage [47, 49].

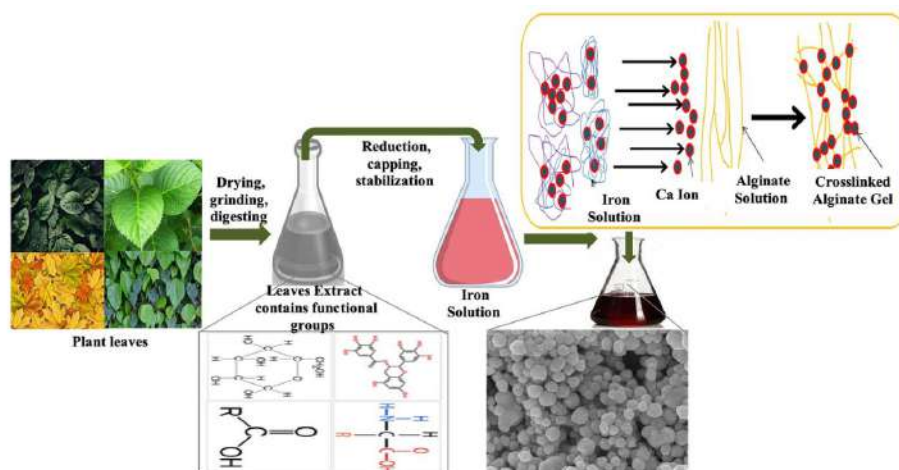


Figure 5.1. Synthesis cycle for plant-mediated nanocomposites: schematic of how plant extracts, rich in phytochemicals such as polyphenols, flavonoids, terpenoids, sugars, and organic acids, act simultaneously as reducing agents that convert dissolved metal ions (e.g., Ag^+ , Au^{3+} , Cu^{2+}) into zero-valent nanoparticles and as stabilizing (capping) agents that prevent aggregation and control particle growth. During the process, functional groups like $-\text{OH}$, $-\text{COOH}$, $-\text{C}=\text{O}$, and $-\text{NH}_2$ coordinate to the nanoparticle surface, forming an organic shell that improves colloidal

stability, tunes surface charge, and can impart additional bioactivity or selective interaction with pollutants. In the context of this manual, the figure illustrates the “green synthesis” route discussed in Chapter 5, showing how renewable plant-derived ligands can replace synthetic reducing and capping agents in the fabrication of nanocomposites for wastewater treatment, thereby aligning materials design with the principles of environmental sustainability and circular bioeconomy. [Cotica, L.F. et al. Green synthesis of bionanocomposites using plant extracts for water and wastewater remediation. In: Bionanocomposites for Wastewater Treatment, Elsevier, 2018, Fig. 2. doi:10.1007/978-981-10-8666-3_1]

5.2. Life Cycle Assessment (LCA) and the Production Paradox

Life Cycle Assessment is the standard tool (ISO 14040) used to measure a system's environmental impact from "cradle-to-grave". In the context of nanocomposites, researchers often face a "Production Paradox" [48, 50]:

- **Energy Intensity of Production:** Nanomaterials often have a much higher cradle-to-gate energy demand than conventional materials. For instance, producing carbon nanotubes (CNTs) via Chemical Vapor Deposition (CVD) can require between 1 and 900 GJ/kg of primary energy, compared to only ~0.2 GJ/kg for aluminum. This is primarily due to the high temperatures (up to 1200°C) and vacuum conditions required for growth [48, 50].
- **Functionality-Driven Savings:** The higher environmental burden of production is often offset during the use phase. Because nanoparticles are typically used in very small amounts (e.g., <5 wt% in a polymer matrix), their high energy intensity is "diluted" within the final device [48].
- **Operational Benefits:** At the device level, the upgraded functionality—such as lightweighting in automobiles or 20-fold increases in water flux for membranes—offers energy-efficient operation that lowers the total life cycle energy demand compared to conventional technologies [48].

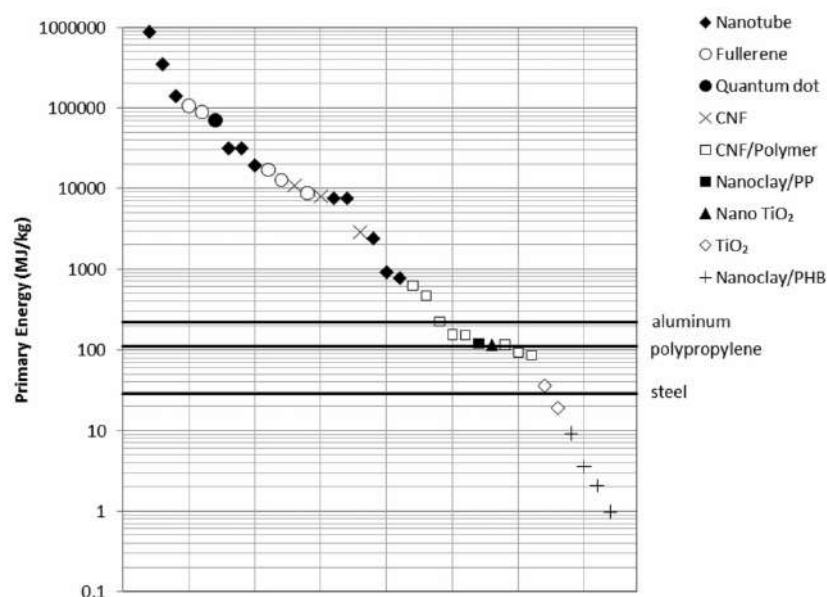


Figure 5.2. Energy demand to produce nanostructured materials vs conventional composites: comparative life cycle assessment showing that many stand-alone nanomaterials (e.g., CNTs, metal oxides, advanced nanofillers) exhibit significantly higher cumulative energy demand per kilogram than bulk polymers, metals, or conventional fillers,

largely due to energy-intensive synthesis, purification, and size-control steps. However, when these nanomaterials are incorporated into composite matrices at low loading fractions (typically < 1–5 wt%), their high “per-kg” energy burden is effectively diluted across the entire composite, while still delivering substantial performance gains such as increased durability, higher efficiency, or reduced use-phase energy. In the context of this manual, the figure underpins the sustainability argument in Chapter 5: by using nanostructured components sparingly but strategically within nanocomposites, it is possible to balance functional benefits in water and wastewater treatment with acceptable life cycle energy and environmental costs, rather than relying on bulk nanomaterials alone. [Kim, H.C. & Fthenakis, V. Life cycle energy and environmental analysis of nanomaterials and their applications in composites. *J. Industrial Ecology*, 2013, 17(4), 528–541, Fig. 1. doi:10.1111/j.1530-9290.2012.00538.x]



Figure 5.3 Circular cradle-to-grave Life Cycle Assessment (LCA) framework for a nanocomposite product: five interconnected stages — Raw Materials extraction → Manufacture (synthesis, fabrication) → Use of Product (water treatment, filtration cycles) → Recycle (regeneration of adsorbent, magnetic recovery) → Waste management (disposal or upcycling) — are evaluated together at the centre in terms of environmental impact categories such as global warming potential (GWP), ecotoxicity, and resource depletion. The circular layout highlights that end-of-life options (regeneration, recycling, magnetic recovery of active phases, or upcycling of spent media) can significantly reduce the overall environmental burden compared to linear, single-use scenarios by lowering demand for virgin raw materials and mitigating waste emissions. In the context of this manual, the figure operationalizes the sustainability concepts introduced in Chapter 5 by showing how nanocomposite-based water treatment technologies should be designed and assessed not only for high removal efficiency, but also for realistic service lifetime, ease of regeneration, and environmentally sound end-of-life management, aligning materials selection and process design with circular-economy principles. [Ramadan, B.S. et al. Circular life cycle assessment of nanocomposite-based water treatment technologies. *Global NEST Journal*, 2024, 26(7), 06216, Fig. 1. doi:10.30955/gnj.006216]

5.3. Safe-by-Design Principles

'Safe-by-Design' (SbD) prioritizes hazard minimization during the early design stage, as mandated by the EU Chemical Strategy for Sustainability and the OECD SSbD framework (2022) [51, 52].

- **Robust Encapsulation:** To prevent secondary pollution, design strategies focus on the stable immobilization of nanoparticles within the composite matrix. For instance, carboxymethyl cellulose-bridged nano-adsorbents have demonstrated ~99.6% stable immobilization over one year, with leaching rates as low as 0.005% [51].

- **Recyclability and Recovery:** A key to sustainability is the ability to recover the material after use. Magnetic nanocomposites (e.g., Fe_3O_4 cores with silica shells) are a model for SbD because they can be easily separated from treated water using an external magnetic field, allowing for up to 10+ cycles of reuse with minimal loss of efficiency [12, 51].
- **End-of-Life Management:** Designing for a "commercial afterlife" involves ensuring that nanocomposites can be regenerated (e.g., through pH adjustment or thermal treatment) to restore their adsorption capacity and recover valuable pollutants like heavy metals [51].
- **Standardization Gap:** As of 2025–2026, standardized leaching test methods for nanocomposites are still absent; the OECD TG 318 (2017) and OECD TG 409 (2024) provide only partial guidance. Physics researchers must contribute to developing these standards [52].

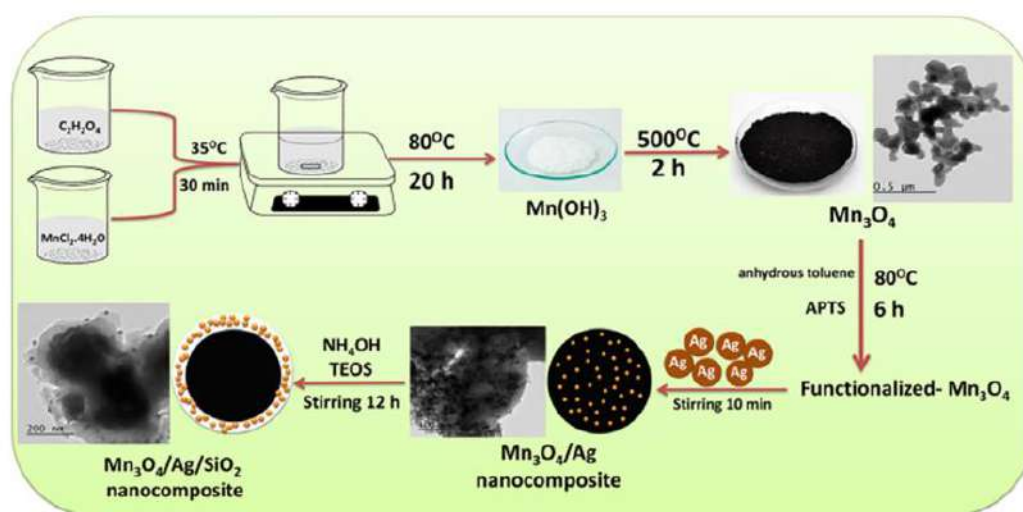


Figure 5.4. Preparation and recovery cycle of a magnetic $\text{Mn}_3\text{O}_4/\text{Ag}/\text{SiO}_2$ nano-catalyst: the photocatalyst is first synthesized by depositing plasmonic Ag and catalytic Mn_3O_4 onto a SiO_2 support, yielding a composite that combines high visible-light activity with superparamagnetic behaviour. During wastewater treatment, the $\text{Mn}_3\text{O}_4/\text{Ag}/\text{SiO}_2$ nanocomposite efficiently degrades organic pollutants under light irradiation, after which the particles are rapidly collected from the treated water using an external magnet, washed, and reused over multiple cycles with only a modest loss of activity. In the context of this manual, the figure exemplifies the design principle from Chapter 5 that nanophotocatalysts for water treatment should be engineered not only for high degradation efficiency but also for facile separation and regeneration, so that environmental benefits from advanced photocatalysis are not offset by difficult recovery or secondary nanoparticle pollution. [Sharshir, S.W. et al. Nanocomposites for water treatment, photocatalysis, and challenges: a systematic review. *Global Challenges*, 2025, 9(10), e00217, Fig. 7. doi:10.1002/gch2.202500217]

Conclusions and Future Perspectives

The development of nanocomposites for environmental and safety applications represents a critical intersection of fundamental physics, materials science, and ecological engineering [3, 51]. As global pollution and resource scarcity escalate, the transition toward high-performance eco-materials is a necessity for global sustainability. The ability to see and manipulate matter on the nanoscale, combined with a deep understanding of atomic-scale interactions, allows for the creation of materials that respond dynamically to environmental stimuli.

- **Fundamental Characterization:** Physics provides essential analytical tools—scanning tunneling microscopy (STM), atomic force microscopy (AFM), SQUID magnetometry, and X-ray photoelectron spectroscopy—to characterize nanoscale structure–property relationships [11, 12].
- **Quantum and Electronic Design:** Physicists engineer electronic band structures (Z-scheme heterojunctions, Schottky barriers) to harness visible light for energy-efficient decontamination [22, 35, 39].
- **Predictive Modeling and AI:** The future of material discovery lies in the integration of computer simulations and Artificial Intelligence (AI) to predict how a material will behave before it is even synthesized, thereby reducing the time and resources wasted in laboratory trials. [35].
- **Bridging Lab to Industry:** While many nanocomposites show success at the lab scale, detailed technical physics studies are required to understand immobilized nanoparticle–host interactions and structure manipulation to guide the design of multifunctional materials for industrial applications [51, 52].

Self-Study Problems

Problem (Chapter 1.2) — TiO₂ nanoparticle bandgap

Using the Brus equation, calculate the bandgap E_g and the corresponding light absorption wavelength λ for an anatase TiO₂ nanoparticle of diameter $d = 5$ nm. Compare with the bulk value ($E_{g,bulk} = 3.2$ eV).

Parameters: $m_e^* = 9 \times 10^{-31}$ kg, $m_h^* = 3 \times m_e^*$, $\epsilon = 86$.

Answer: $E_g \approx 3.52$ eV; $\lambda \approx 352$ nm (blue-shifted from 388 nm for bulk).

Problem (Chapter 1.3) — Blocking temperature of Fe₃O₄

Estimate the blocking temperature T_B for Fe₃O₄ nanoparticles ($K = 11$ kJ/m³) for three diameters: $d = 5, 10, 20$ nm. Use $\tau_0 = 10^{-9}$ s, $\tau_m = 100$ s. Conclude which particles are superparamagnetic at room temperature ($T = 293$ K).

Answer: $T_B(5 \text{ nm}) \approx 2.1$ K; $T_B(10 \text{ nm}) \approx 16.5$ K; $T_B(20 \text{ nm}) \approx 132$ K. All three are superparamagnetic at RT ($T \gg T_B$).

Problem (Chapter 3.1) — Carrier separation efficiency η_{sep}

Calculate η_{sep} for two photocatalysts: (a) bulk TiO₂ ($\tau_r = 10^{-10}$ s, $D = 10^{-12}$ m²/s, $r = 50$ μ m); (b) TiO₂ nanoparticle ($\tau_r = 10^{-10}$ s, $D = 10^{-12}$ m²/s, $r = 5$ nm). Compare results and explain why nanoparticles show superior photocatalytic efficiency.

Answer: $\eta_{sep}(bulk) \approx 2 \times 10^{-7}$ (negligible); $\eta_{sep}(nano) \approx 0.96$ (96%). Dramatic improvement due to $\tau_d = r^2/D$ reduced from 2.5 s (bulk) to 25 ps (nano).

Problem (Chapter 4.3) — Stokes–Einstein diffusion of nanoparticles in air

Calculate the diffusion coefficient D for nanoparticles of $d = 10$ nm in air at 37°C. Cunningham factor $C_c = 22$. $\eta_{air} = 1.9 \times 10^{-5}$ Pa·s. Compare with D for $d = 1$ μ m ($C_c \approx 1.16$). Comment on the significance for occupational health.

Answer: $D(10 \text{ nm}) \approx 5.2 \times 10^{-8}$ m²/s; $D(1 \mu\text{m}) \approx 2.7 \times 10^{-13}$ m²/s. Nanoparticles diffuse $\sim 200,000 \times$ faster $\rightarrow$ dramatically higher alveolar deposition rate.

List of Abbreviations and Acronyms

Abbreviation	Full Form
AFM	Atomic Force Microscopy
AI	Artificial Intelligence
AQY	Apparent Quantum Yield
BET	Brunauer–Emmett–Teller (surface area analysis method)
CB	Conduction Band
CIMC	Calcon-Imprinted Magnetic Chitosan (nanoparticles)
CNF	Carbon Nanofiber
CNT	Carbon Nanotube
CVD	Chemical Vapor Deposition
DDA	Discrete Dipole Approximation (computational electromagnetic method)
DLVO	Derjaguin–Landau–Verwey–Overbeek (colloidal stability theory)
DPV	Differential Pulse Voltammetry
EDL	Electrical Double Layer
ENM	Engineered Nanomaterial
ET	Extrathoracic (respiratory tract region)
FFP3	Filtering Face Piece class 3 (European standard for respiratory protection)
GWP	Global Warming Potential
GO	Graphene Oxide
HGMS	High-Gradient Magnetic Separation
HRTM	Human Respiratory Tract Model (ICRP)
ICRP	International Commission on Radiological Protection
ICP-MS	Inductively Coupled Plasma Mass Spectrometry
ISO	International Organization for Standardization
IUPAC	International Union of Pure and Applied Chemistry
LCA	Life Cycle Assessment
LOD	Limit of Detection
LSPR	Localized Surface Plasmon Resonance
MD	Molecular Dynamics (simulation)

MF	Microfiltration
MNP	Magnetic Nanoparticle
MS	Magnetic Separation
MWCNT	Multi-Walled Carbon Nanotube
nAg	Nano-Silver (silver nanoparticles)
NC	Nanocomposite
NF	Nanofiltration
NIR	Near-Infrared
OECD	Organisation for Economic Co-operation and Development
PPE	Personal Protective Equipment
PZC	Point of Zero Charge
PVDF	Polyvinylidene Fluoride
QD	Quantum Dot
QSE	Quantum Size Effect
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals (EU regulation)
RO	Reverse Osmosis
ROS	Reactive Oxygen Species
SbD	Safe-by-Design
SPE	Screen-Printed Electrode
SPR	Surface Plasmon Resonance
SQUID	Superconducting Quantum Interference Device
SSA	Specific Surface Area
SSbD	Safe and Sustainable by Design (OECD/EU framework)
STM	Scanning Tunneling Microscopy
S/V	Surface-to-Volume Ratio
SWCNT	Single-Walled Carbon Nanotube
TEM	Transmission Electron Microscopy
UF	Ultrafiltration
UV	Ultraviolet
VB	Valence Band
VOC	Volatile Organic Compound
WHO	World Health Organization
XPS	X-ray Photoelectron Spectroscopy

XRD	X-ray Diffraction
ZVI	Zero-Valent Iron

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