Water Challenges from the Process Systems Engineering Perspective

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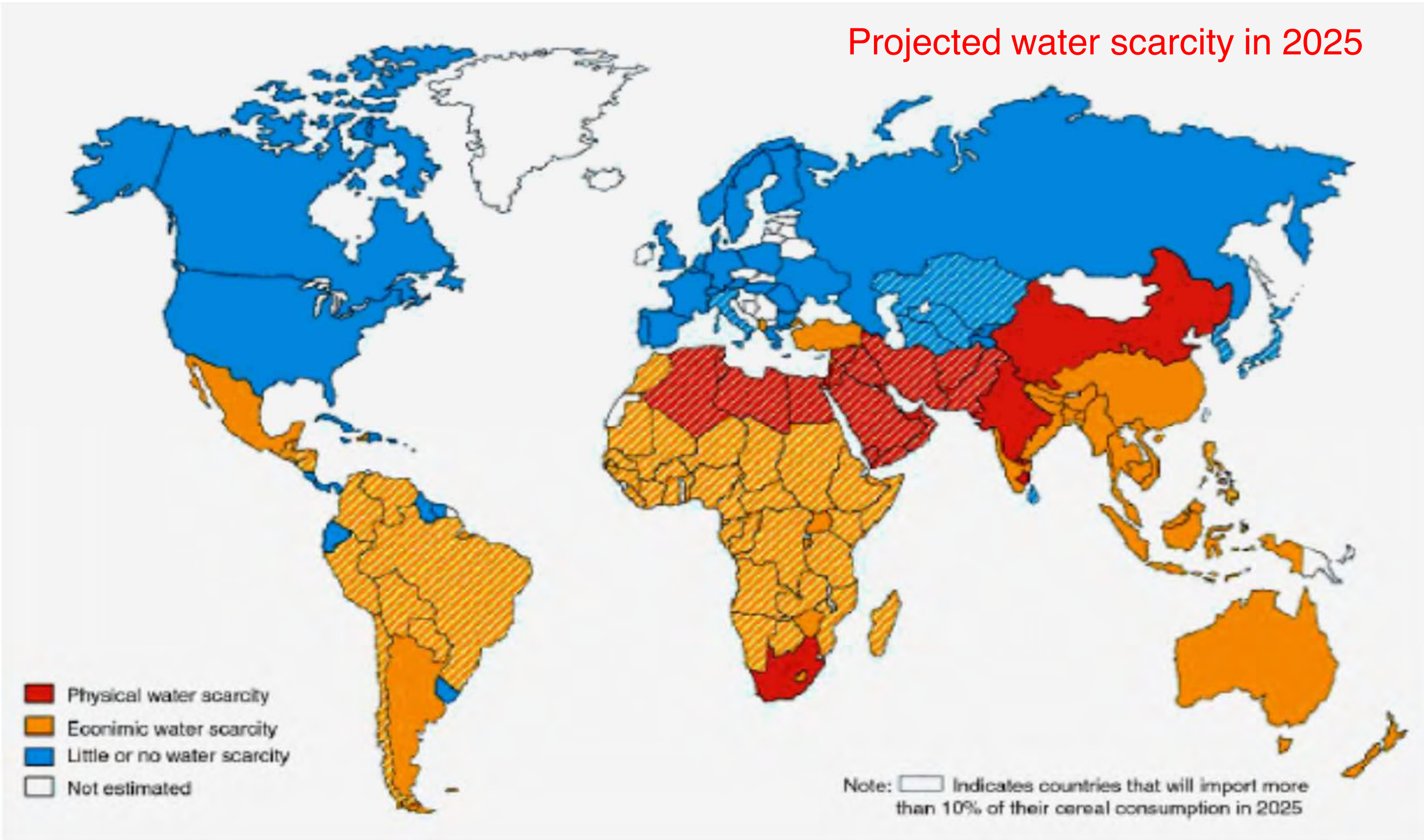
FIPSE4 Symposium

Porto Carras, Chalkidiki, June 25-27, 2018

Foreword

- Water is the most important asset, and potable water supply is a basic human necessity. However, we are far from meeting global demands.
- Demand escalates due to population growth, global climate change, and water-quality deterioration.
- Although two-thirds of the Earth's surface is water, only 0.3% is freshwater consumable by the 7.3 billion humans that populate the Earth. The remaining 99.7% is comprised of saltwater, glacial bodies, and water vapor unusable by humans.



Water Challenges from the PSE Perspective

Length and Time Scales of Water Related Challenges

1. Length: Global, Continent, Country, Region, City

   Time: Long Term Planning, Years

   Challenges: Water Resource Systems Planning and Management

2. Length: Region, City, Plant

   Time: Years, Months, Days, Hours

   Challenges: Water Treatment and Purification Facilities

3. Length: Process, Equipment, Component **– Microscale, Nanoscale**

   Time: Hours. Minutes, Seconds

   Challenges: Nanotechnology-based Water Purification Methods

Process Systems Engineering Can Contribute to the Solution of the Above Challenges

Water Resource Systems Planning- Management

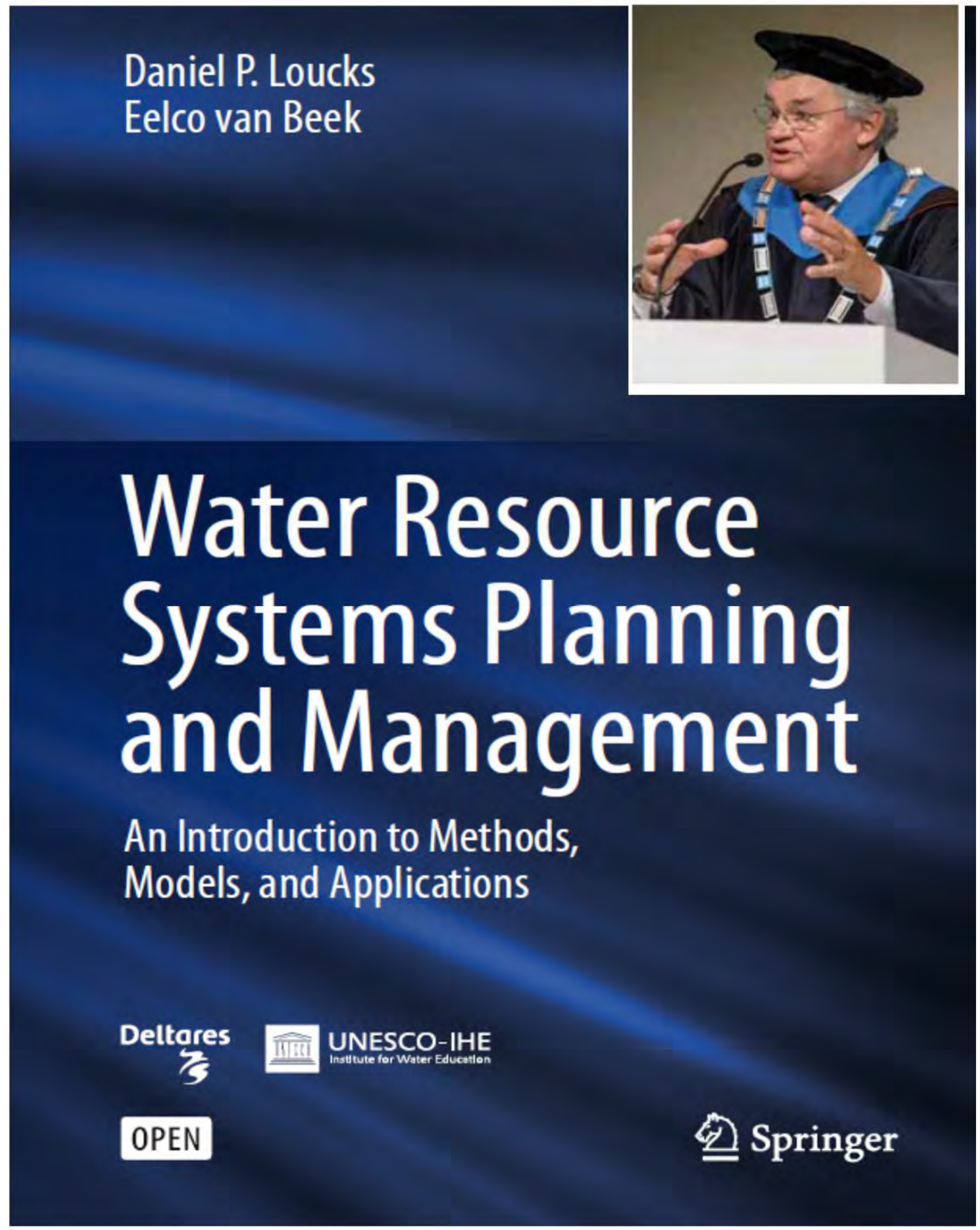
Life on this planet depends on water. Most of our economic activities consume water.

All the food we grow, process and eat requires water. Much of our waste is transported and assimilated by water.

The importance of water to our well-being is beyond question. Our dependence on water will last forever.

Note that in 1975 water availability stood at around 13,000 m^3 per person per year, it has now dropped to 6000 m^3; meanwhile water quality has also severely deteriorated.

This is by itself a very disturbing development.



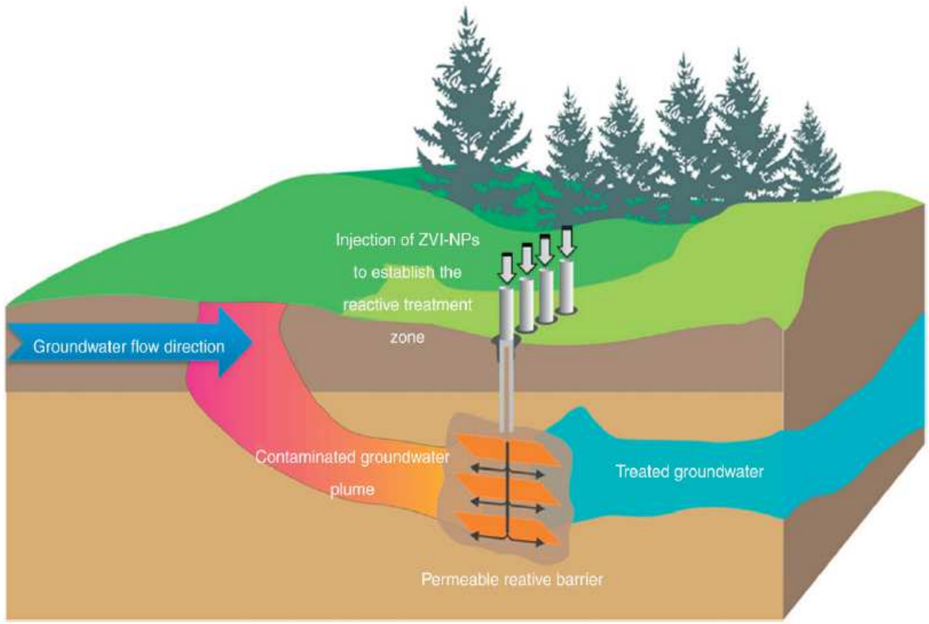
So, What is the Problem?

- The answer is simply that water, although plentiful, is not distributed as we might wish. There is often too much or too little, or what exists is too polluted or too expensive. A further problem is that the overall water situation is likely to further deteriorate as a result of global changes.

- This is a result not only of climatic change but also of other global change drivers such as population growth, land use changes, urbanization and migration from rural to urban areas, all of which will pose challenges never before seen.

- For example, while population growth in the twentieth century increased threefold—from 1.8 to 6 billion people—water withdrawal during the same period increased six fold!

- That is clearly unsustainable.



Water Challenges from the PSE Perspective

- Integrated Water Resources Management: The concept of integrated water resources management (IWRM) is the response to the growing pressure on our water resources systems caused by growing populations and socioeconomic developments. Water shortages and deteriorating water quality have forced many countries in the world to reconsider their development policies with respect to the management of their water resources.

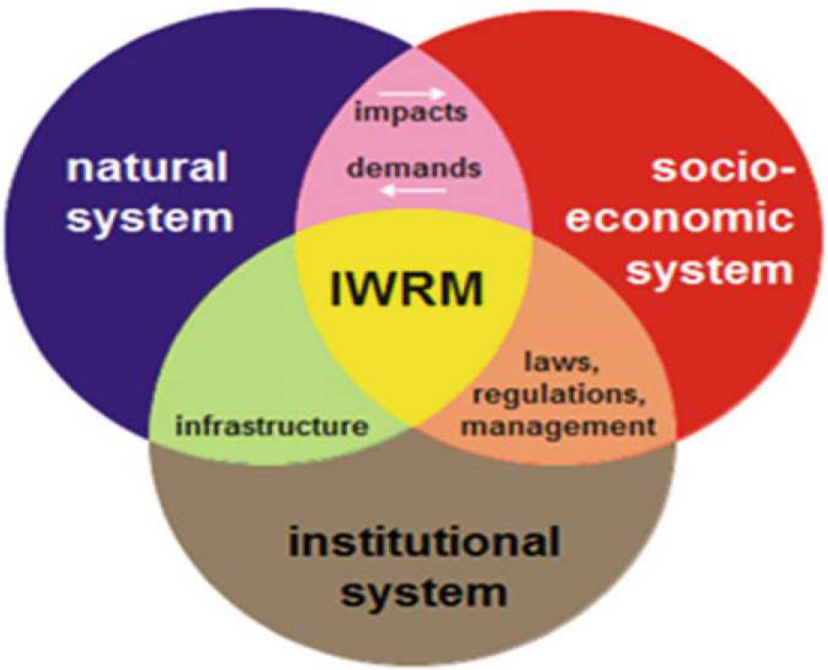


Figure 1: Interactions among the natural, administrative, and socioeconomic water resource subsectors and between them and their environment

✓ Definition of IWRM

IWRM is a process which promotes the coordinated development and management of water, land, and related resources, in order to maximize the resultant economic and social welfare in an equitable manner without compromising the sustainability of vital ecosystems.

Water Challenges from the PSE Perspective

- Water Security and the Sustainable Development Goals

  - The World Economic Forum has identified Water Security as one of the biggest global economic development issues. Water Security was defined by UN-Water (2013) as

  - The capacity of a population to safeguard sustainable access to adequate quantities of acceptable quality water for sustaining livelihoods, human well-being, and socio-economic development, for ensuring protection against water-borne pollution and water-related disasters, and for preserving ecosystems in a climate of peace and political stability.

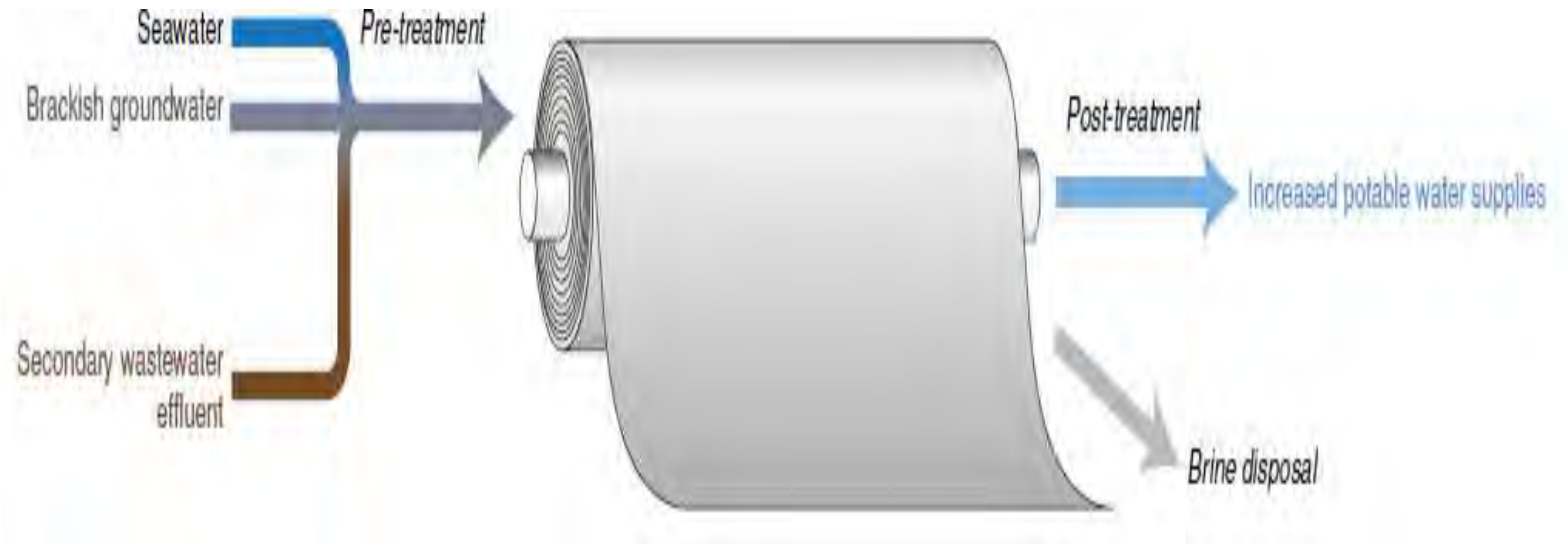
Definition of Sustainability

The need for new approaches to urban water and resource management is being driven by the need for sustainability, defined as:

Table 1. Triple Bottom Line Urban-Water and Resource-Management Sustainability Goals

Sustainability Area	Goal
Economy	• Financially stable utilities with enough resources to maintain their infrastructure.
Environment	• Locally sustainable water supply (recharge exceeds net withdrawal). • Energy-neutral system (or positive if possible), with minimal chemical consumption. • Responsible nutrient management that minimizes dispersal to the aquatic environment.
Society	• Access to clean water and appropriate sanitation for all.

Achieving Sustainability Goals



- Desalination membranes used in high-membrane-area spiral-wound modules.

  - Even though technological advances continue to reduce these energy requirements, they will always be higher than for treating fresh wastewater, because the solids content of wastewater (1,000 mg/L) is much smaller than of seawater (35,000 mg/L).

Tools for Water Management and Sustainability

Software tools are available for:

(1) More efficient capture and local use of storm water to help conserve local water resources;

(2) Improved water conservation for reducing water consumption without compromising standards of living;

(3) The reclamation and reuse of wastewater;

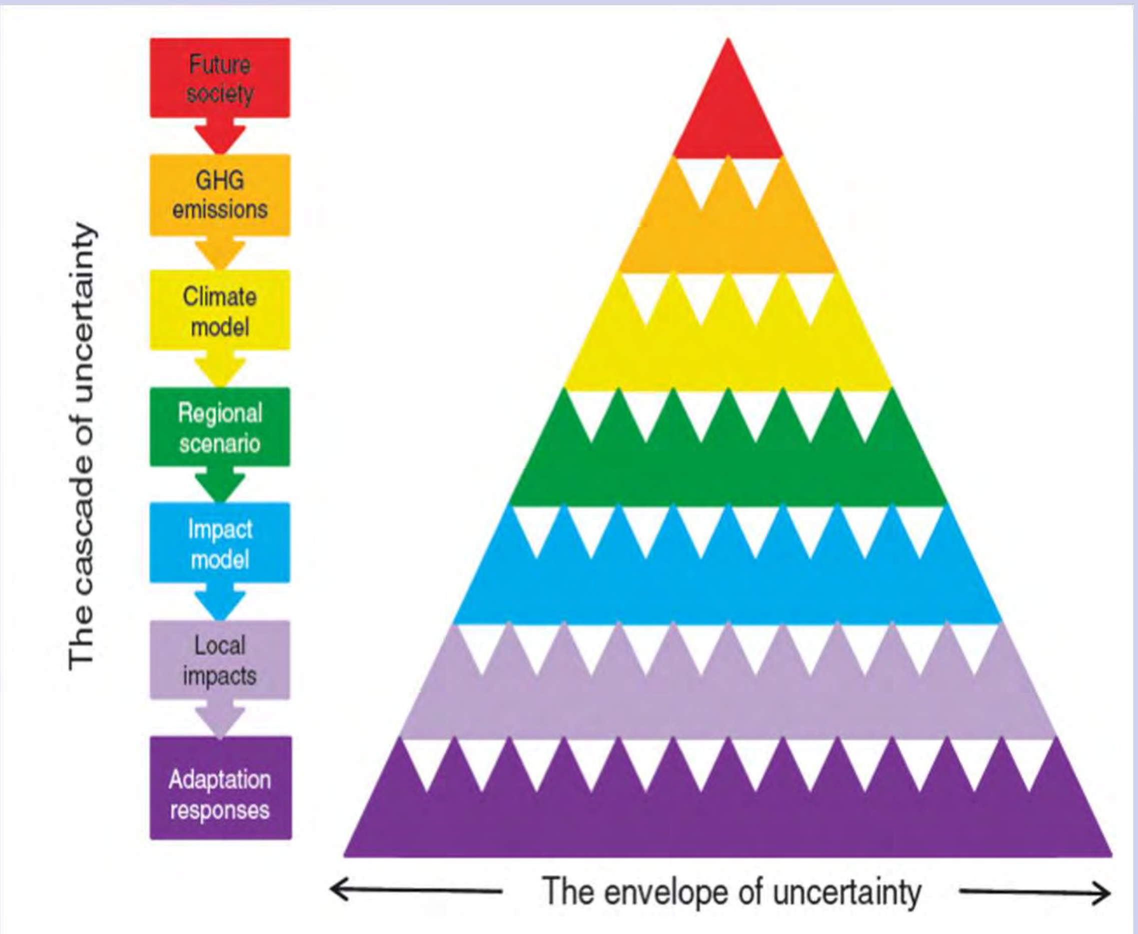
(4) The management and extraction of energy from the wastewater stream;

(5) The recovery of nutrients; and

(6) The separation of specific waste water sources.

Models Uncertainty

Traditional approaches **amplify** or **hide** uncertainty



Source: Wilby & Dessai, 2010, *Weather*

- ✓ Models not developed for adaptation purposes but for testing hypotheses about greenhouse gas mitigation.
- ✓ Low confidence, especially for quantitative purposes.
- ✓ Little agreement across models, scenarios.
- ✓ Often result in a series of "no regret" options.
- ✓ Stakeholders often feel disempowered by process, which is often experienced as deterministic.

Source: AGWA, "Caveat Adaptor," 2013

Technologies for Water Sustainability-Management

Many technologies are available to facilitate the implementation of systems such as the one shown in Figure 2 and for improving decentralized and centralized water and resource management (Table 2). The goal is to conserve local water resources for meeting a variety of local needs.

Tools	Centralized Systems	Decentralized Systems
Storm water management and rainwater harvesting		Permeable pavements, green roofs, rain gardens, etc.
Water conservation	New technologies and behavioral changes	
Water reclamation and reuse	Treatment for potable uses and reuse (direct and indirect)	Treatment for potable uses and non-potable reuse
Energy management	Anaerobic digestion, combustion, microbial fuel cells	Capture of heat energy, microbial fuel cells
Nutrient recovery	Land application of biosolids, struvite recovery	
Source separation	Treatment of kitchen, black, and yellow wastewater	Supply potable and non-potable water; treatment of kitchen, black, and yellow wastewater

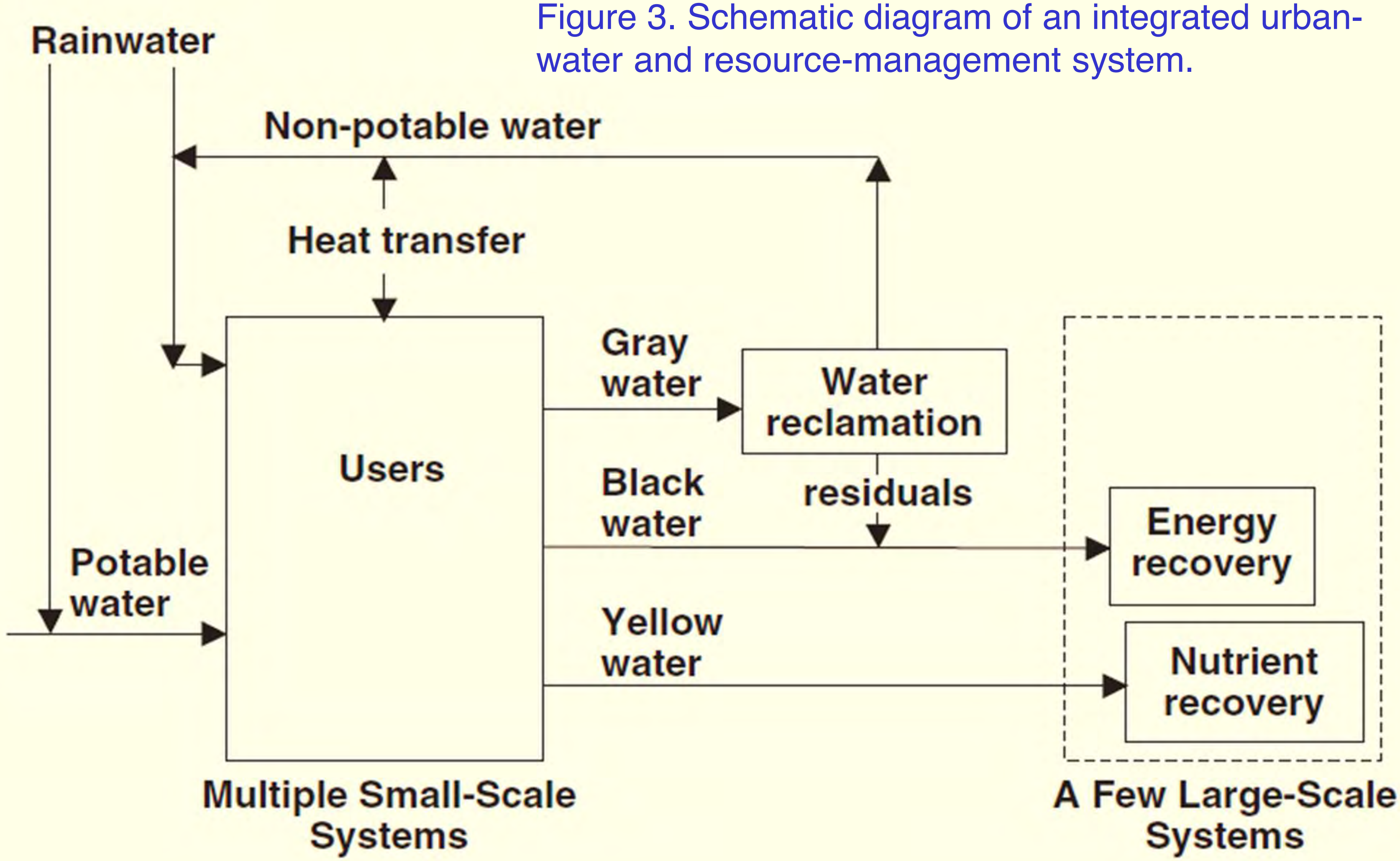


Figure 3. Schematic diagram of an integrated urban-water and resource-management system.

Technologies for Sustainable Water Systems

- Laundry and bath water (typically referred to as gray water), which contain very few pollutants, constitute the largest component of urban wastewater. Because of its low-pollutant content, gray water requires only a modest degree of treatment to become reusable non-potable water.

- Most of the organic matter (quantified as the five-day biochemical oxygen demand, or BOD_5) is contained in toilet and kitchen waste (typically referred to as black water). The wastewater flow associated with these components is quite small, suggesting that the black-water fraction can be used efficiently for energy production.

- The majority of nutrients is found in the urine stream (typically referred to as yellow water). When energy management and nutrient recovery are combined with source separation, energy can be efficiently produced and extracted from the wastewater stream, along with nutrient recovery.

Industrial Process Water Treatment and Reuse

I&EC research
Industrial & Engineering Chemistry Research

Article

pubs.acs.org/IECR

Industrial Process Water Treatment and Reuse: A Framework for Synthesis and Design

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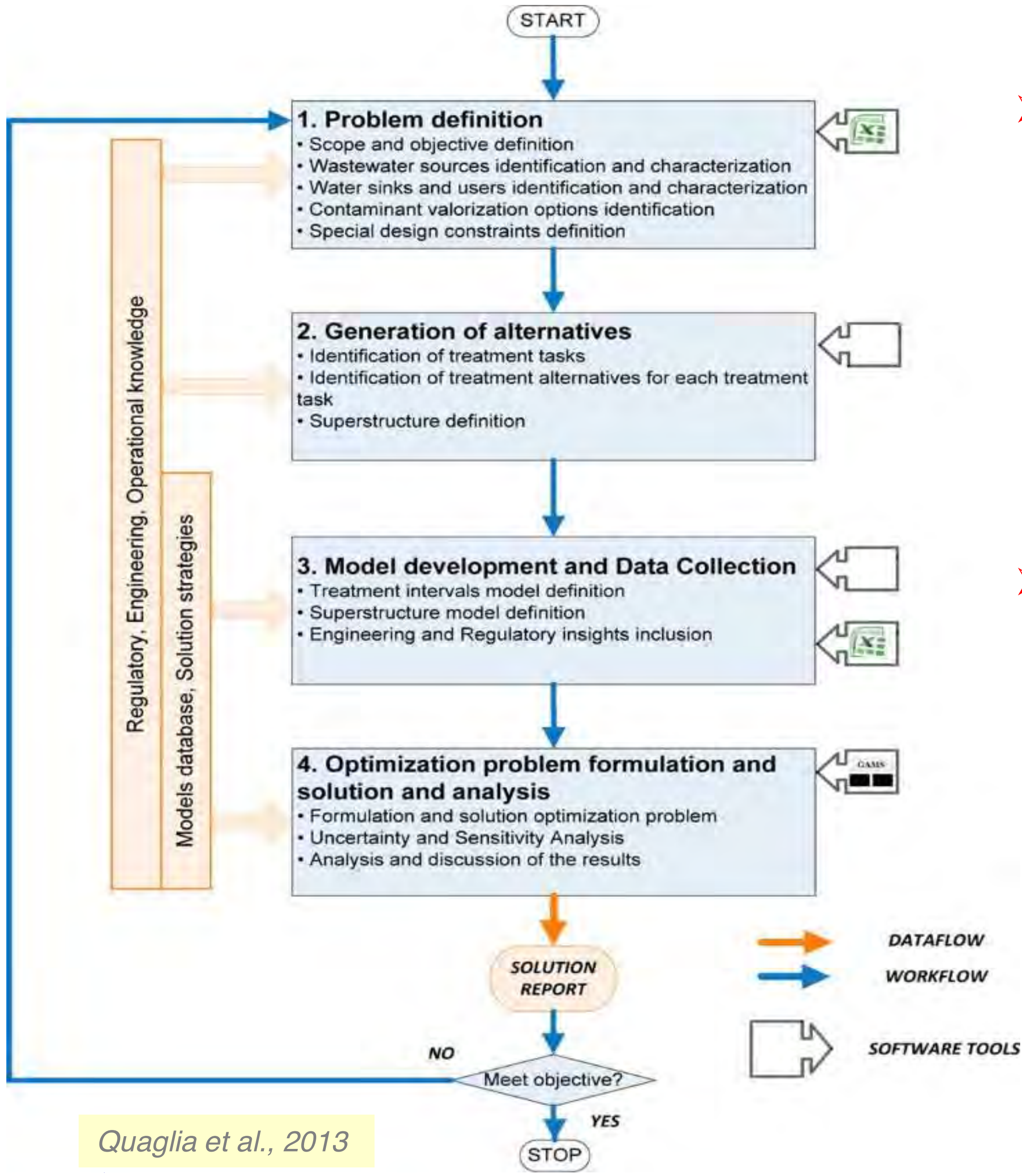
Supporting Information

ABSTRACT: Mathematical optimization has shown the potential to contribute to industrial water management, through the development of the solution methods needed for optimization-based design of wastewater treatment and reuse networks (also called water networks). Nevertheless, the application of this approach is still limited to motivating examples lacking the ability to handle problems with complexity of industrial relevance. To address this challenge, in this contribution, we focus on the integration of wastewater engineering concepts and models, together with optimization methods and solution algorithms. To this end, we propose a computer-aided framework for the design of water treatment and reuse networks. In the framework, optimization methods, problem analysis tools and wastewater engineering knowledge are integrated in a computer-aided environment, in order to facilitate the formulation and solution of the design problems with fair complexity representative of industrial applications. The framework is demonstrated through the solution of a case study dealing with the treatment and reuse of water effluent produced by an oil refinery. The problem is solved, and a win−win solution is identified, allowing a reduced water footprint, and the treatment costs are identified.

Process Systems Engineering Approach

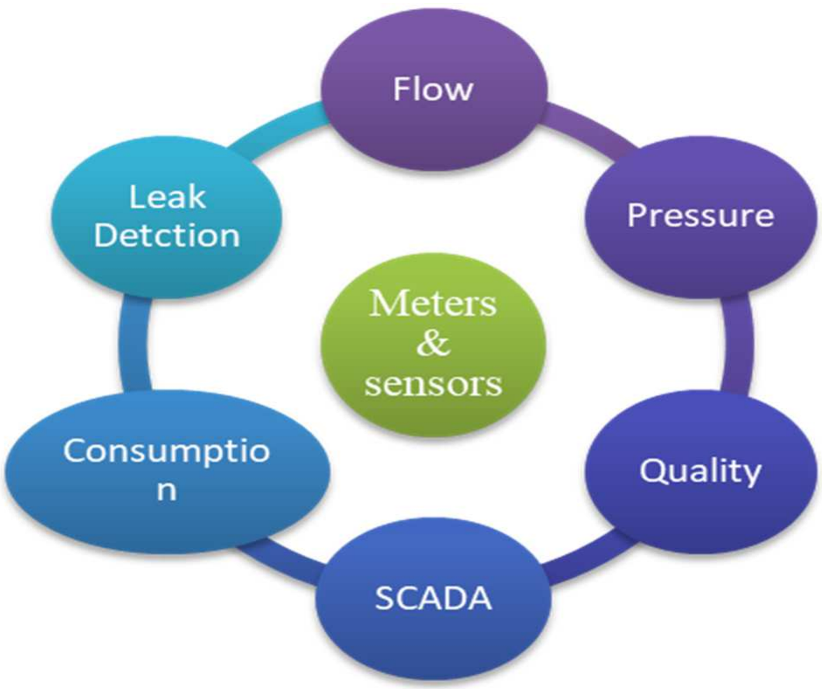


Quaglia et al., 2013

- Mathematical optimization contributes to industrial water management, through the development of the solution methods needed for optimization-based design of wastewater treatment and reuse networks.
- Optimization methods, problem analysis tools and wastewater engineering knowledge are integrated in a computer-aided environment, in order to facilitate the formulation and solution of the design problems with fair complexity representative of industrial applications.

Meters and Sensors

- Meters and sensors are currently being intensively applied to regulate different activities of water distribution systems such as hydraulic pressure and flow, water quality, head losses, and water and energy consumptions.
- The major aim of water utilities is to convey water from one place to another without any losses, saving water and avoiding any damages caused by leaking water.



Types of meters and sensors that have been developed for effective and sustainable water resource management

Supervisory Control and Data Acquisition (SCADA)

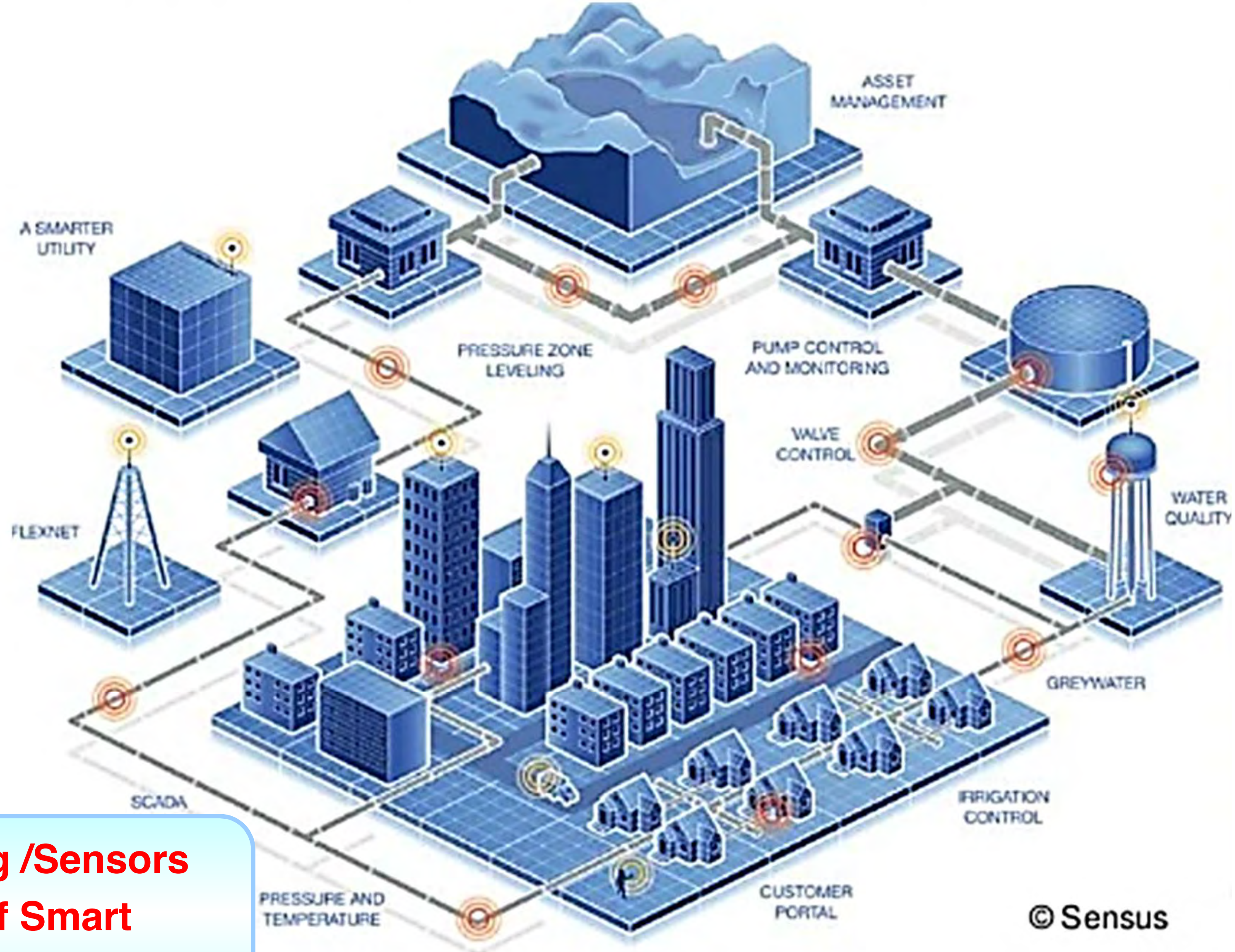
Meters and Sensors - SCADA

SCADA includes, but is not limited to, software packages that can be incorporated into a system of hardware and software to improve the safety and efficiency of the operation of these large processes.

In general, SCADA systems perform main functions like the acquisition of data through the sensors, the transmission of the acquired data between a number of remote sites, the data presentation through the central host computer and the control of the data at the operator terminal or workstations. These systems usually consist of the following subsystems:

- Remote terminal units (RTUs) or programmable logic controllers (PLCs) which interface with the sensors in the process;
- A communication infrastructure connecting the remote terminal units with the supervisory system or central host computer;
- A supervisory (computer) system, gathering (acquiring) data on the process and sending commands (control) to the process, sometimes called a SCADA centre, master station, master terminal unit, or MTU;
- A communication system to support the use of operator workstations;
- Standard human machine interface (HMI) software or man machine interface (MMI) software system, which is used to provide the central host and operation terminal application of SCADA, support the communication system and monitor and control remotely located field data interfaces devices.

Smart Water Networks



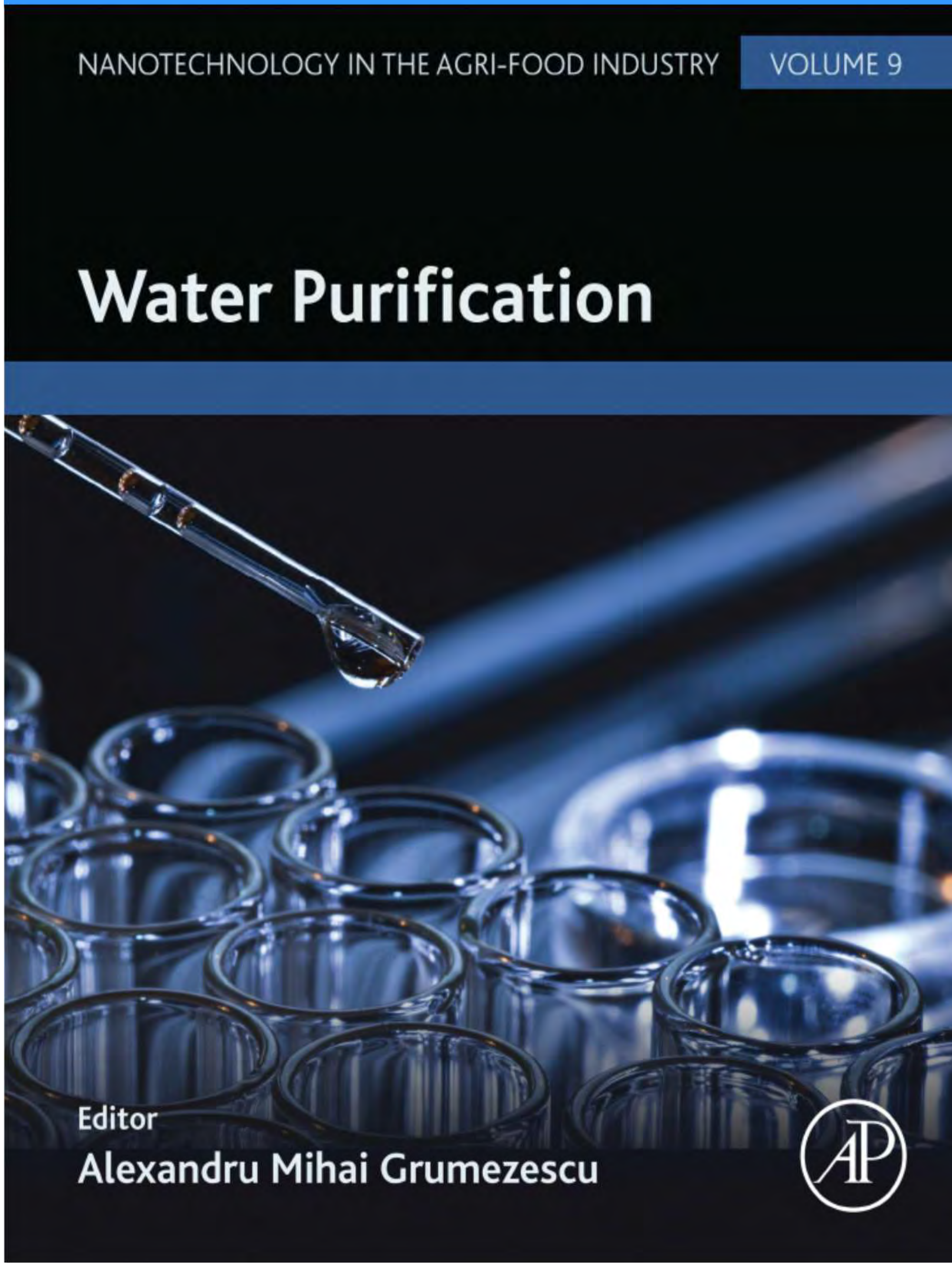
Smart Metering /Sensors are the heart of Smart Water Networks

Water Challenges from the PSE Perspective

PSE tools for addressing present water resource systems planning and management challenges

1. Water Resource Systems Modeling
2. Models for Identifying and Evaluating Alternatives
3. Optimization Models and Methods
4. Data-Fitting, Evolutionary, and Qualitative Modeling
5. Modeling Uncertainty
6. System Sensitivity and Uncertainty Analysis
7. Performance Criteria
8. Water Quality Modeling and Prediction
9. Hardware and Software Sensors
10. River Basin Modeling
11. Urban Water Systems

Challenges in Water Purification

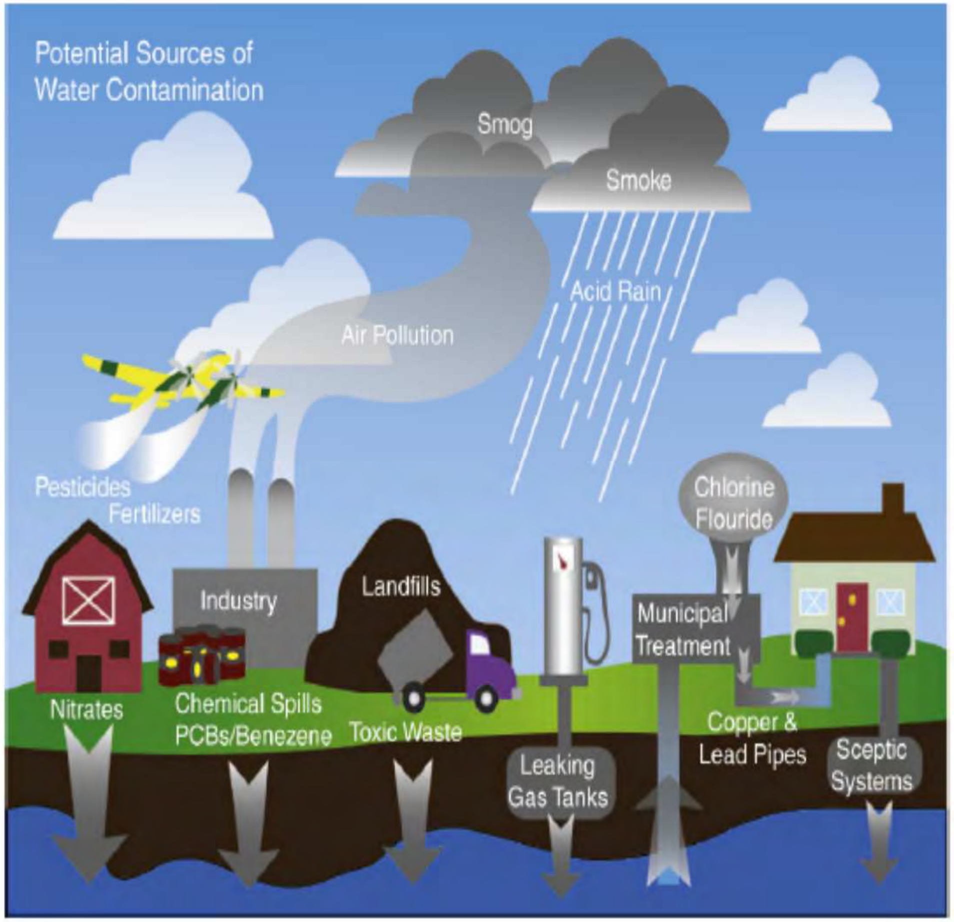


- Improving water quality provides social and economic benefits both to developed and developing countries. Adequate water purification approaches could bring lower costs, a safer environment, and industry and also a huge benefit for human health.

- In recent years, the use of nanostructured materials in developing novel water purification approaches bring numerous advantages over conventional methods previously employed for water purification. From the design of nanoporous membranes to functional nanoparticles and nanosensors, the science of nanosized materials offers now a sustainable alternative for the removal of main pollutants, such as arsenic, bacteria, organic materials, nitrates, salinity, and viruses from most water sources.

Water Contaminants

- Available technologies for water treatment are reaching their limits in providing sufficient quality to meet human and environmental needs.
- New organic contaminants (e.g. pesticides, hormones, drugs, various aromatic compounds, etc.) cannot be removed by conventional chemical, biological, and photolytic processes.
- Most of these contaminants are carcinogenic and cause the formation of dangerous disinfection by-products (DBPs).
- Finally, some microbial pathogens are resistant to conventional disinfectants, such as chlorination and ozonation.



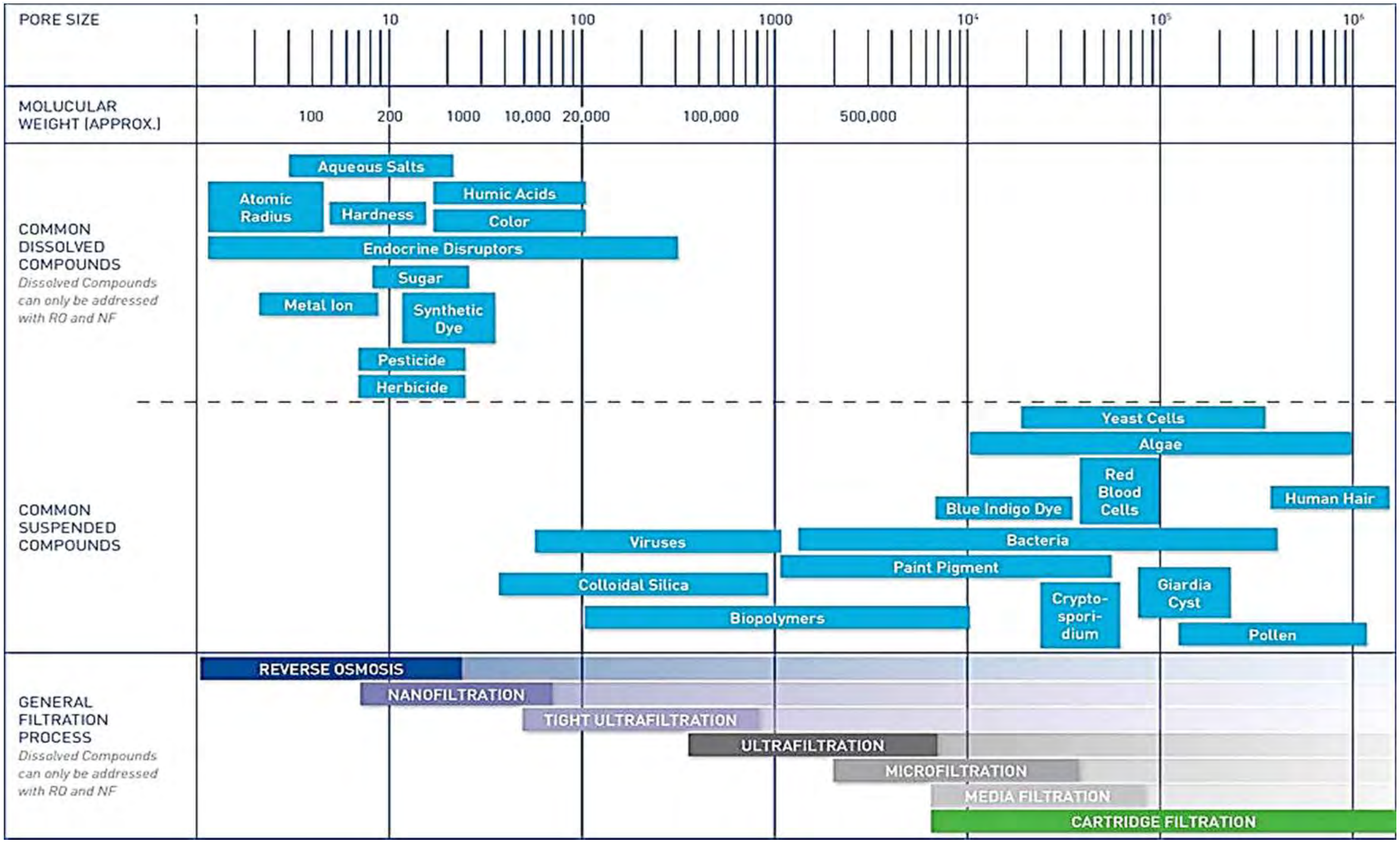
Conventional Methods & Limitations

Conventional Methods	Limitations
Distillation	Most contaminants require high amounts of energy and water. Pollutants with boiling point >100℃ are difficult to remove.
Chemical transformation	Excess reagents are required. The product may be a low-quality mixture and cannot be released into environment. Inactive in harsh conditions. Not highly selective method.
Coagulation and flocculation	Complex and less-efficient method requiring alkaline additives to achieve optimum pH.
Biological treatment	Microorganisms are sensitive to environmental factors and difficult to control. Intermediates damage the microbial cells. Not cost effective. Time consuming.
Ultraviolet treatment	Expensive method, inactivated by water cloudiness and turbidity. Ineffective for heavy metals and other nonliving contaminants removal.
Reverse osmosis	Removes minerals from water which is unhealthy, and the treated water will be acidic. It cannot remove volatile organics, chemicals, chlorine, chloramines and pharmaceuticals. Requires high energy input.
Nanofiltration	Expensive method that requires high energy input, and pretreatment. Limited retention for salts and univalent ions. Membrane fouling and limited lifetime.
Ultrafiltration	Does not remove dissolved inorganics. Requires high energy. Susceptible to particulate plugging and difficult to clean.
Microfiltration	Cannot remove nitrates, fluoride, metals, sodium, volatile organics, color, and so on. Requires regular cleaning. Membrane fouling. Less sensitive to microbes, especially virus.
Carbon filter	Cannot remove nitrates, fluoride, metals, sodium, and so on. Clogging occurs with undissolved solids. Susceptible to mold. Requires frequent changing of filters.

Water Purification, 2017

Traditional Methods

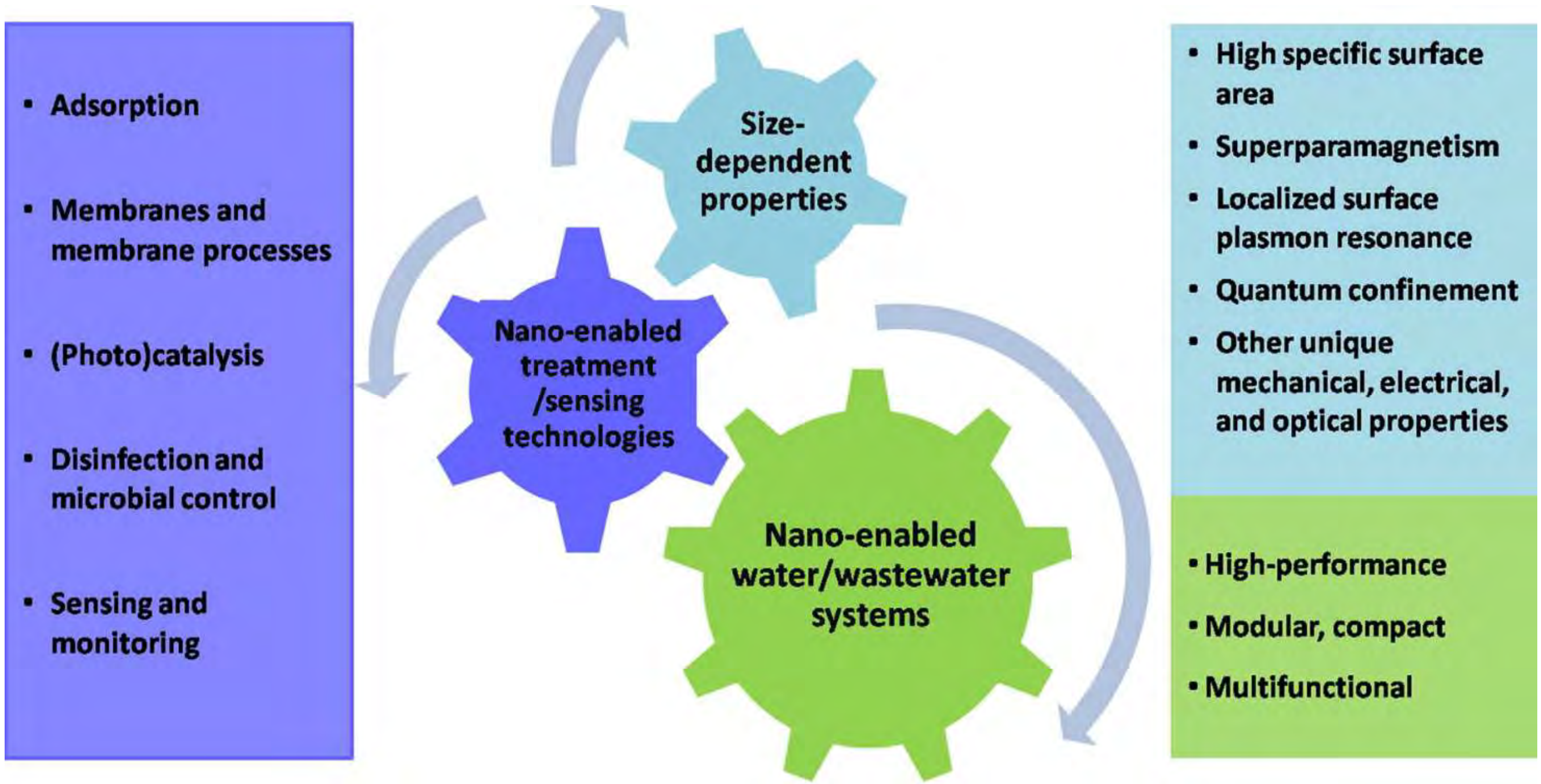
- For the removal of the various contaminants, several methods, such as activated carbon adsorption, ozonation, UV radiation and membrane filtration have been developed.



- However, these methods are normally non-selective.

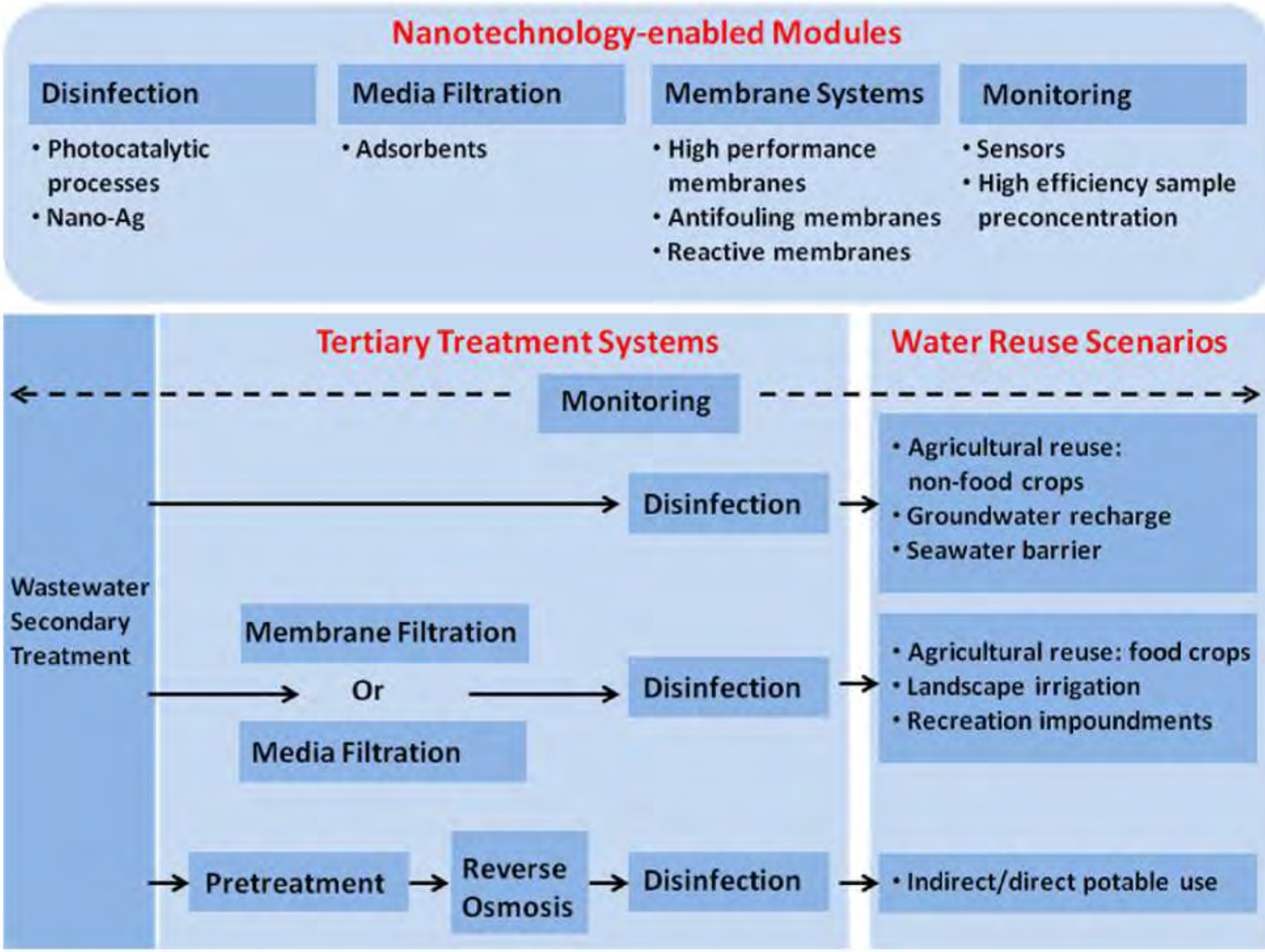
Nanotechnology-Aided Water Purification

- Nanotechnology offers opportunities to develop next-generation water supply systems.
- The extraordinary properties of nanomaterials (e.g., high surface area, photosensitivity, catalytic & antimicrobial activity, electrochemical, optical, and magnetic properties, and tunable pore size and surface chemistry) provide useful features for many applications.
- These applications include sensors for water quality monitoring, specialty adsorbents, solar disinfection/decontamination, and high performance membranes.



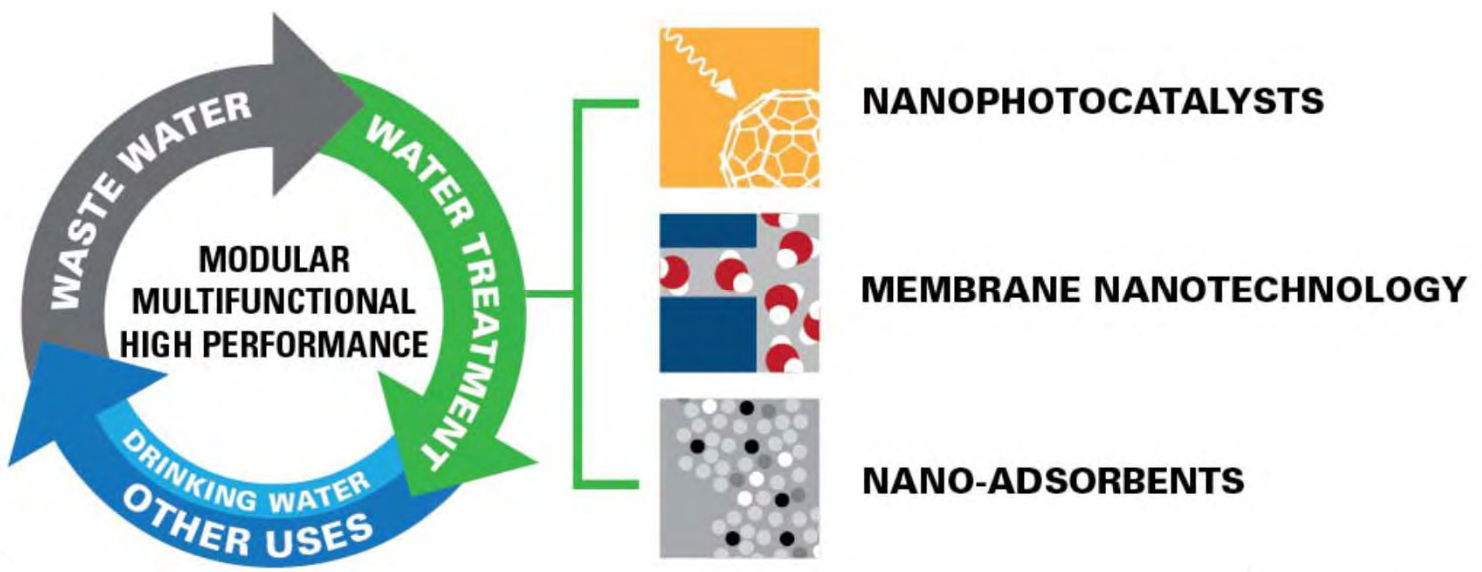
Nanotechnology in Waste Water Treatment

Wastewater tertiary systems with nanotechnology-enabled modular design for differential water reuse scenarios



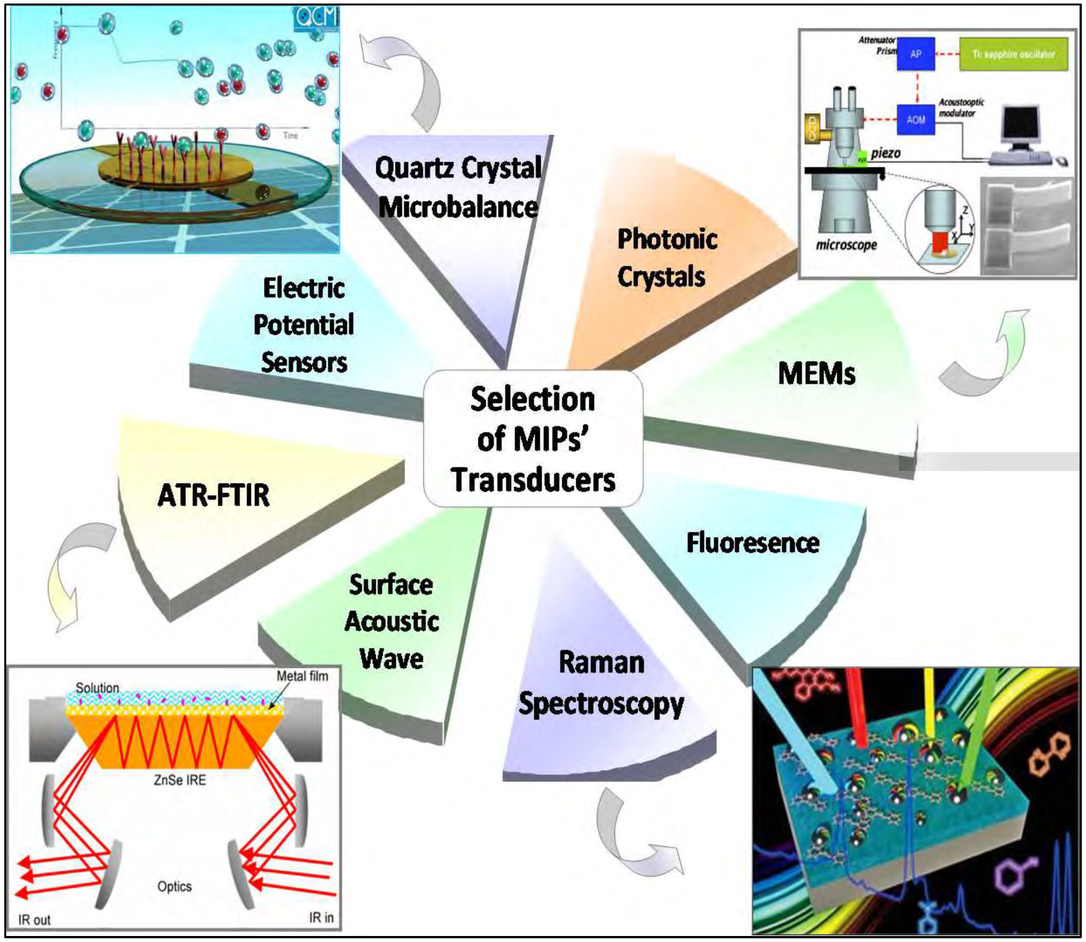
Nanotechnology-based Water Purification

Nanomaterial	Properties/Applications
Nanoadsorbents	• High specific surface and very good adsorption capacity. • Used to remove organic and inorganic contaminants, and bacteria.
Nanometals and nanometal oxides	• Exhibit high specific surface area and short intraparticle diffusion distance. Compressible without change in the surface area, abrasion resistant, magnetic, and photo catalytic in nature. • Used to remove heavy metals and radionuclides. • Used in media filters, slurry reactors, powders, and pellets.
Membranes and membrane process	• Highly reliable and mostly automated process. • Applied in all fields of water and waste water treatments.
Photocatalysis	• Photocatalytic activity in UV and possibly visible light range, low human toxicity, high stability, and low cost.
Disinfection and microbial control	• Strong and wide-spectrum antimicrobial activity, low toxicity to humans, ease of use.



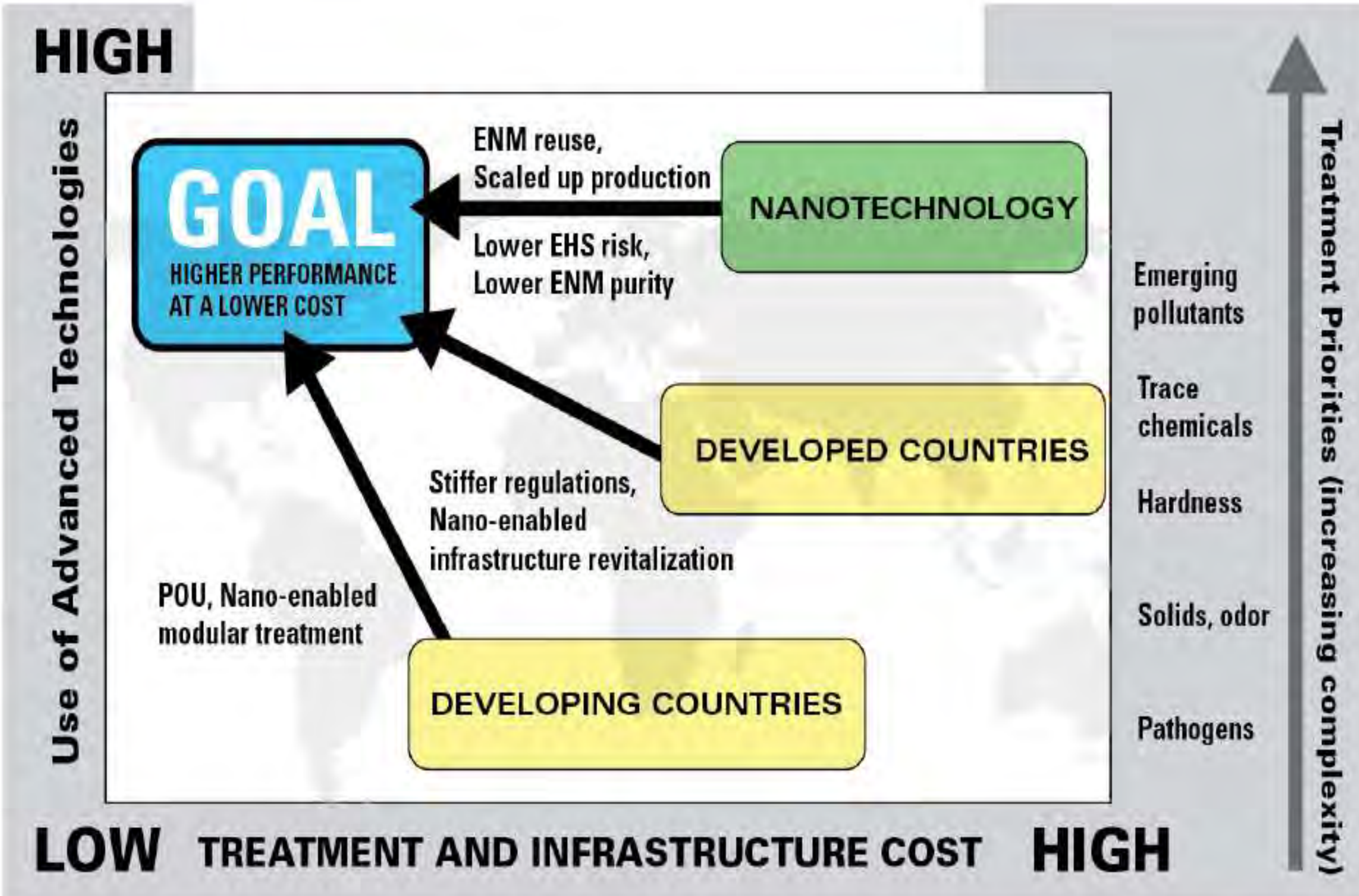
Monitoring and Control Systems

- Research on a new generation of sensor and system-control technologies is ongoing.



- Molecular imprinting for sensor applications and environmental monitoring of contaminants.

Conceptual Improvements to Water Treatment



WSSTP

WssTP is the Water Supply and Sanitation Technology Platform. WssTP was initiated by the European Commission in 2004 for Research and Technology Development in the water industry and was transformed into an independent legal entity under Belgian Law in 2007. WssTP was reconfirmed as one of the best-performing European Technology Platforms (ETPs) in line with the new ETP2020 strategy. **The mission of WssTP includes the following:**

- Foster collaborative, innovative and integrated European Research and Technologies Development
- Ensure the European Growth and Competitiveness of the Water Sector
- Provide Global answers to Global Challenges for the next generations
- Address the challenges of an integrated and sustainable management of water resources

EU & US Initiatives

The European Innovation Partnership on Water (EIP Water) is an initiative within the EU 2020 Innovation Union.

The EIP Water facilitates the development of innovative solutions to address major European and global water challenges, which cannot be addressed or solved with current or business-as-usual approaches and technologies.

At the same time, the EIP Water supports the creation of market opportunities for these innovations, both inside and outside of Europe.

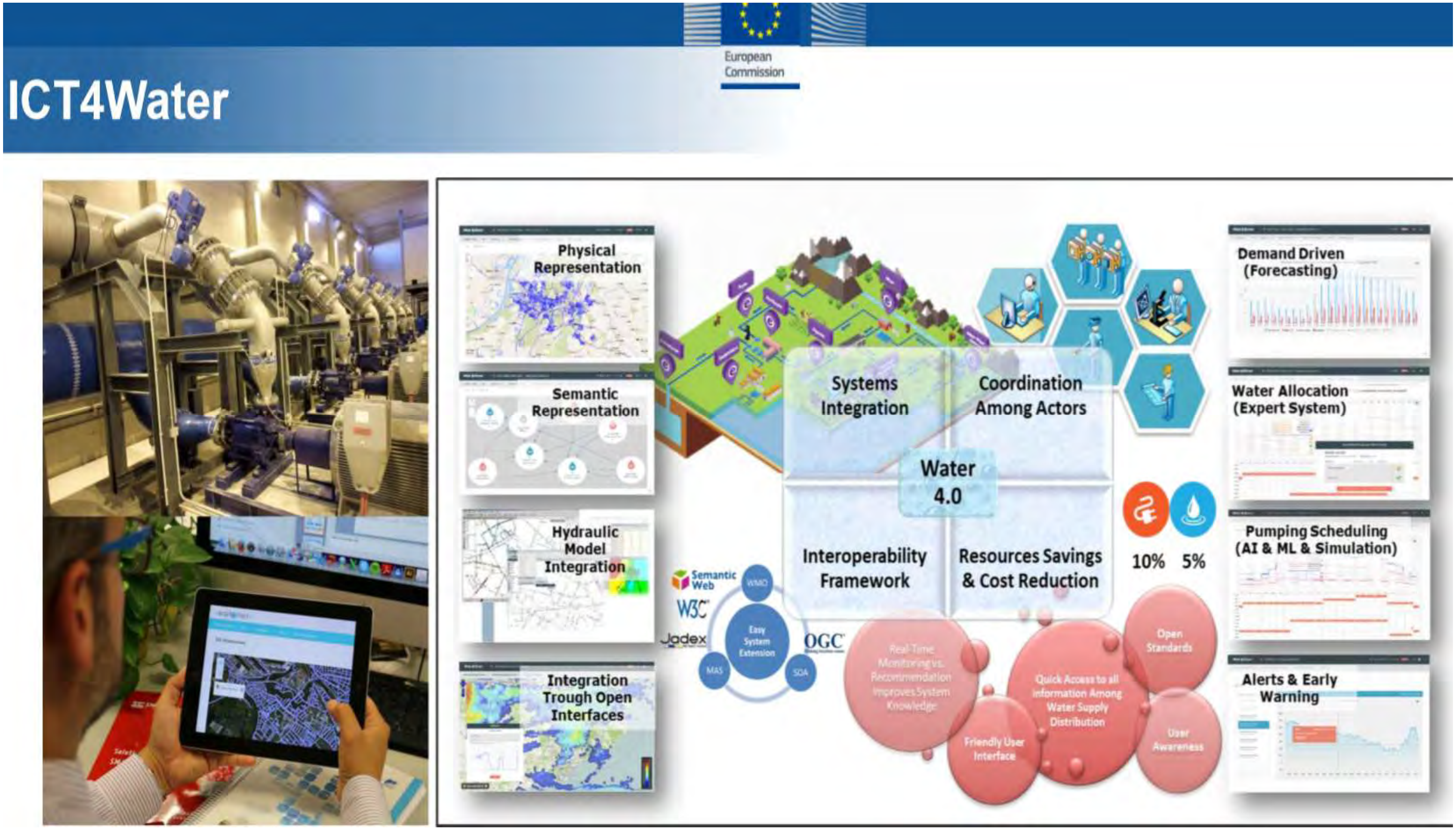
EIP Water Online Market Place

Boosting opportunities – Innovating water

EPA research supports efforts under the Clean Water Act and Safe Drinking Water Act.

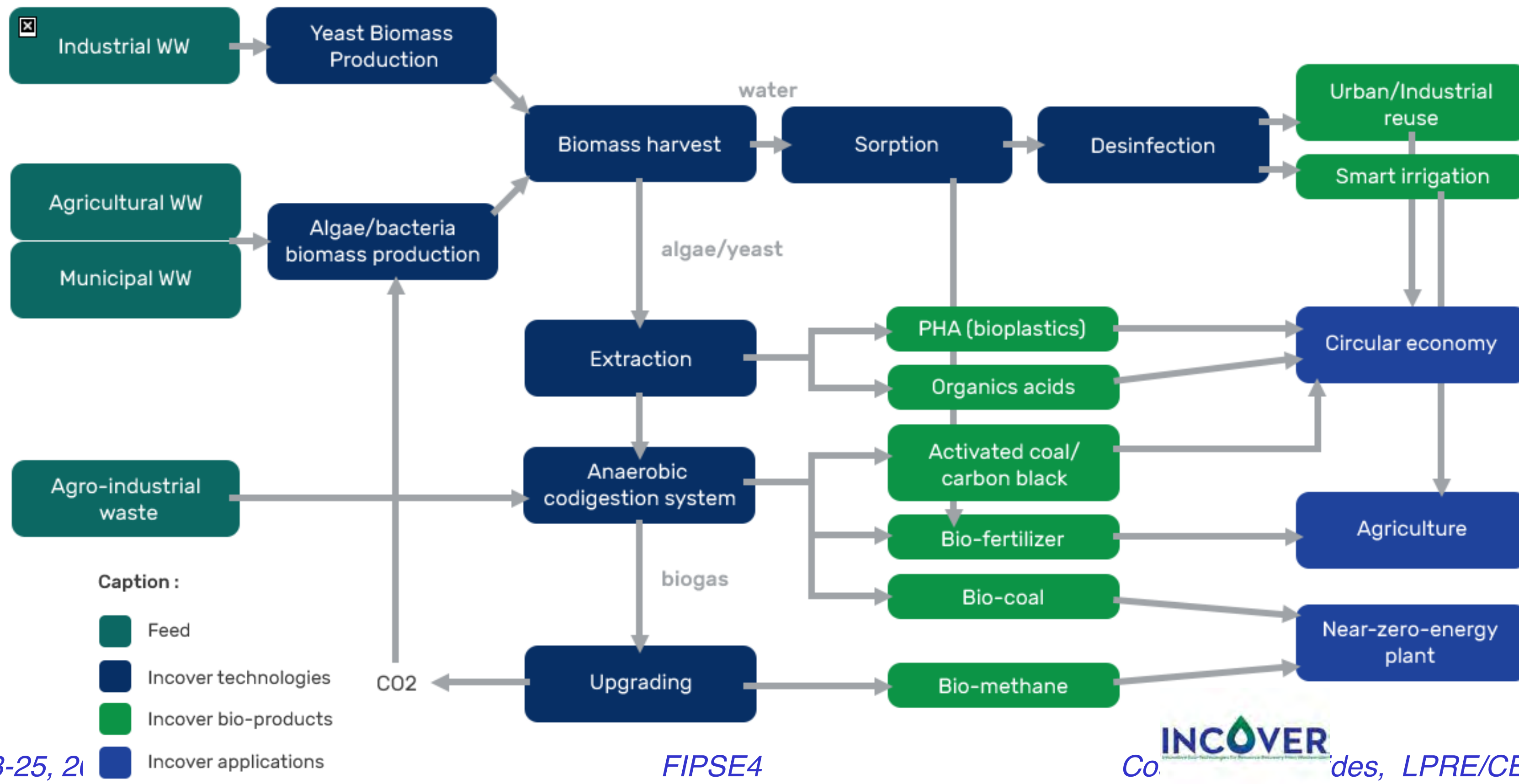
EPA United States Environmental Protection Agency

ICT4WATER


European Commission
ICT4Water
Physical Representation
Semantic Representation
Hydraulic Model Integration
Integration Trough Open Interfaces
Systems Integration
Coordination Among Actors
Water 4.0
Interoperability Framework
Resources Savings & Cost Reduction
10%
5%
Semantic Web
W3C
Jadex
OGC
Easy System Extension
WMO
MAS
SOA
Open Standards
User Awareness
Friendly User Interface
Demand Driven (Forecasting)
Water Allocation (Expert System)
Pumping Scheduling (AI & ML & Simulation)
Alerts & Early Warning

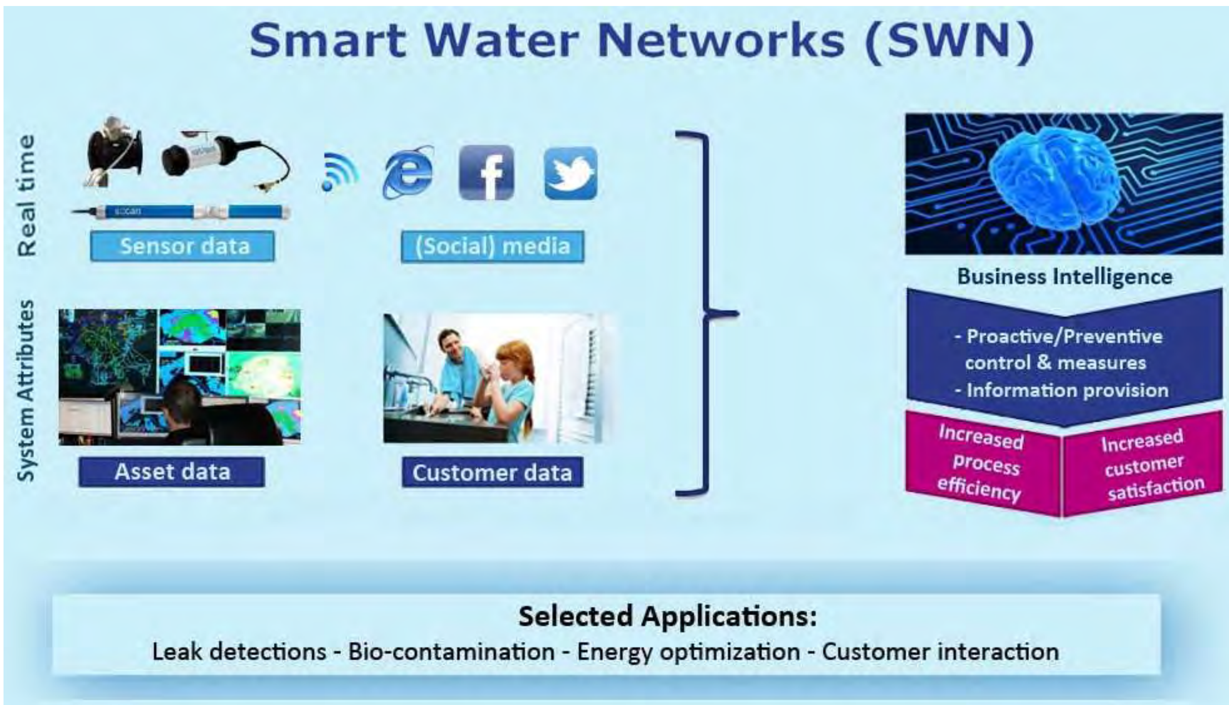
INCOVER EU Project

- INCOVER concept: to move wastewater treatment from being primarily a sanitation technology towards a bio-product recovery industry and a recycled water supplier.
- Added-value plants will generate benefits from wastewater through the following three solutions:
  - ✓ Bio-production (bio-plastics and organic acids) via microalgae/bacteria and yeast biotechnology;.
  - ✓ Near-zero-energy plant providing upgraded bio-methane via pre-treatment and anaerobic co-digestion systems
  - ✓ Chemical recovery (N, P) and reclaimed water via adsorption, biotechnology based on wetlands systems and hydrothermal carbonisation.



SW4EU Project

- For water quality management a combination of generic and specific sensors are a promising solution (less data, less sensors, less investments and costs; maintenance).
  - ✓ Optiqua EventLab generic screening sensor: the sensor measures differences in water quality online based on refractive index;
  - ✓ Specific S::Can spectrometry sensor: The sensor measures turbidity, Nitrate, Colour and organic parameters (Total Organic Carbon and Dissolved Organic Carbon) online based on absorption;
  - ✓ Specific Intellisonde sensor from Intellitect: the sensor measures flow, temperature, free chlorine, monochloramines, dissolved oxygen, pH, ORP, conductivity, color, turbidity, pressure, ISE online based on differences in potential;
  - ✓ Generic Mycometer biologic sensor: the sensor measures biologic activity based on enzyme activity;
  - ✓ Aqua Explorer generic sensor for biologic activity: the sensor measures biologic activity based on antibodies.

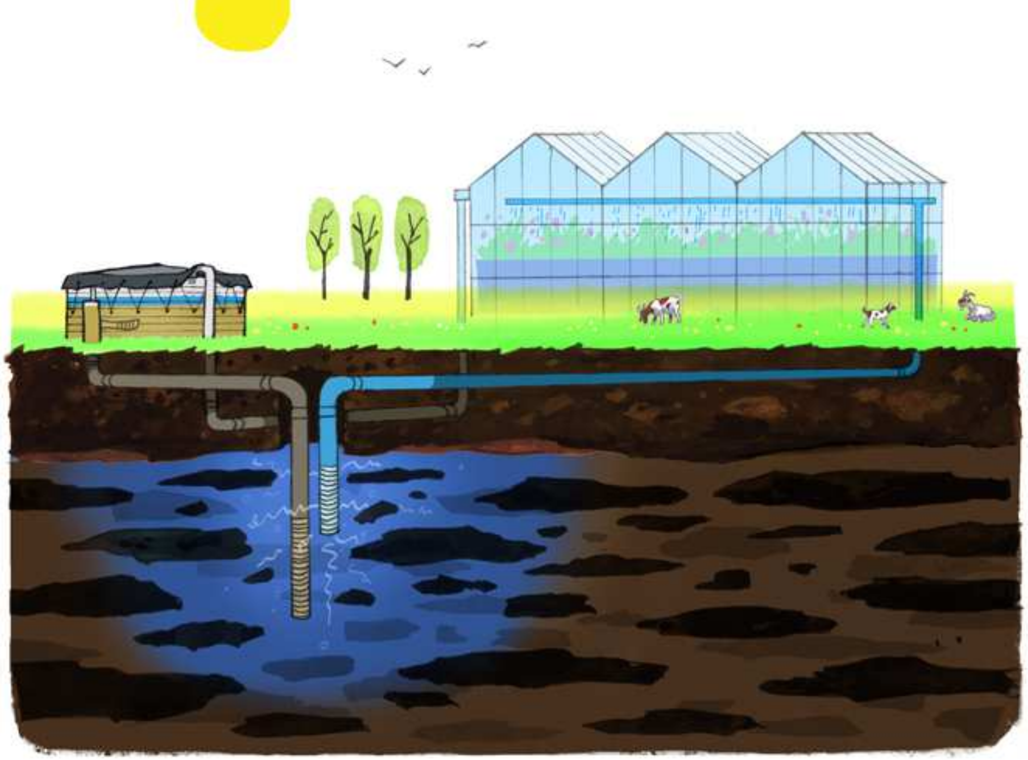


SW4EU

SUBSOL H2020 Project

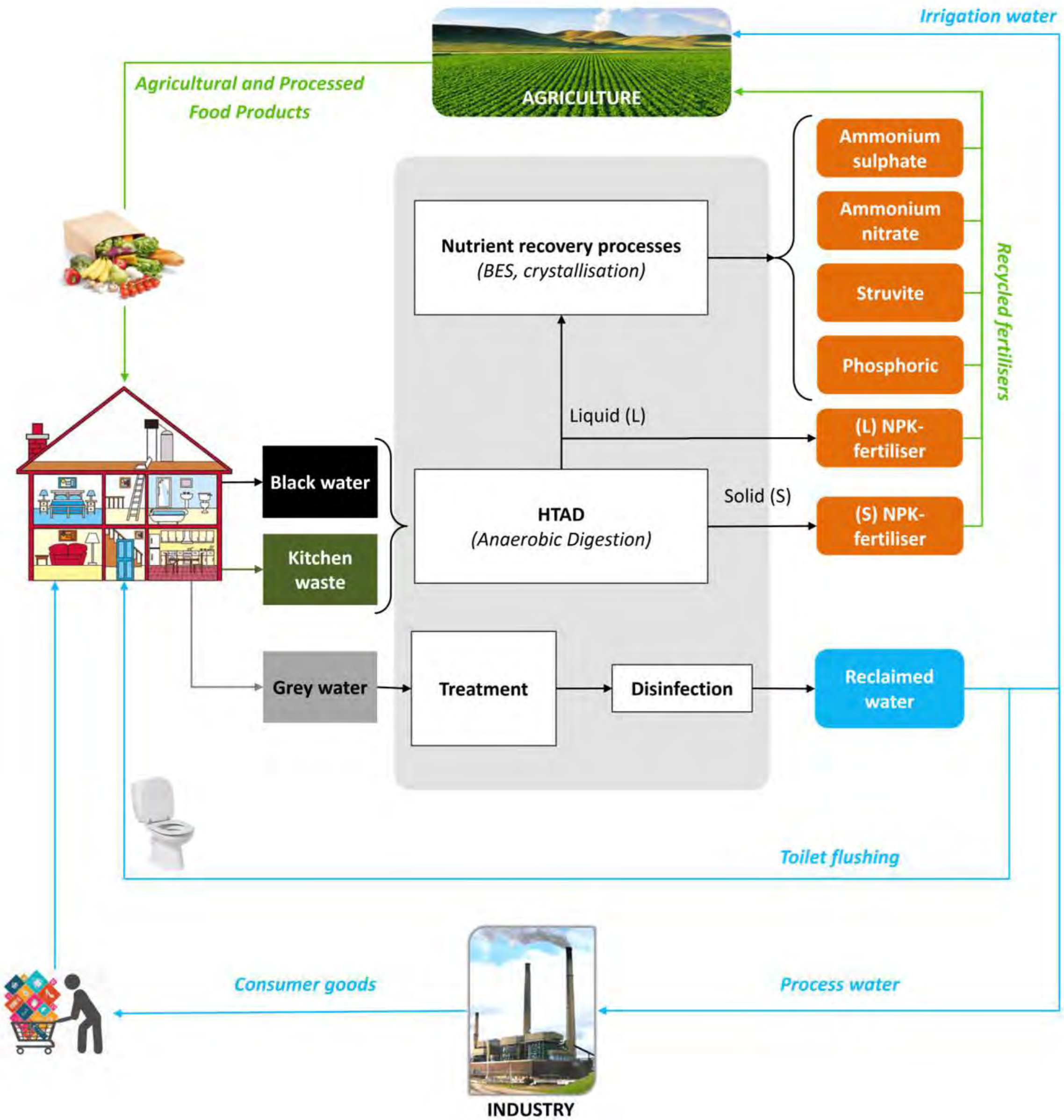
Bringing coastal SUBsurface water SOLutions to the market

- SUBSOL targets a market breakthrough of SWS as robust answers to freshwater resources challenges in coastal areas, by demonstration, market replication, standardization and commercialization.
- The route to market includes business cases, market scans and capacity building in selected regions in Europe (Mediterranean, Northwestern Europe) and worldwide (USA, Brazil, China, Vietnam).



Run4Life H2020 Project

- Run4Life proposes a radical new technological concept for wastewater treatment and nutrient recovery. It is based on source-separated collection of domestic wastewaters and kitchen waste, with each flow receiving optimal treatment for resource recovery and subsequent safe reuse.
- The different collected flows are black water (wastewater from toilets), grey water (other domestic wastewater, e.g. from showers and washing machines) and organic kitchen waste.
- The resources to be recovered from the waste(water) streams are nutrients (N&P), clean water and energy.



Nanotechnology Enabled Water Treatment (NEWT)

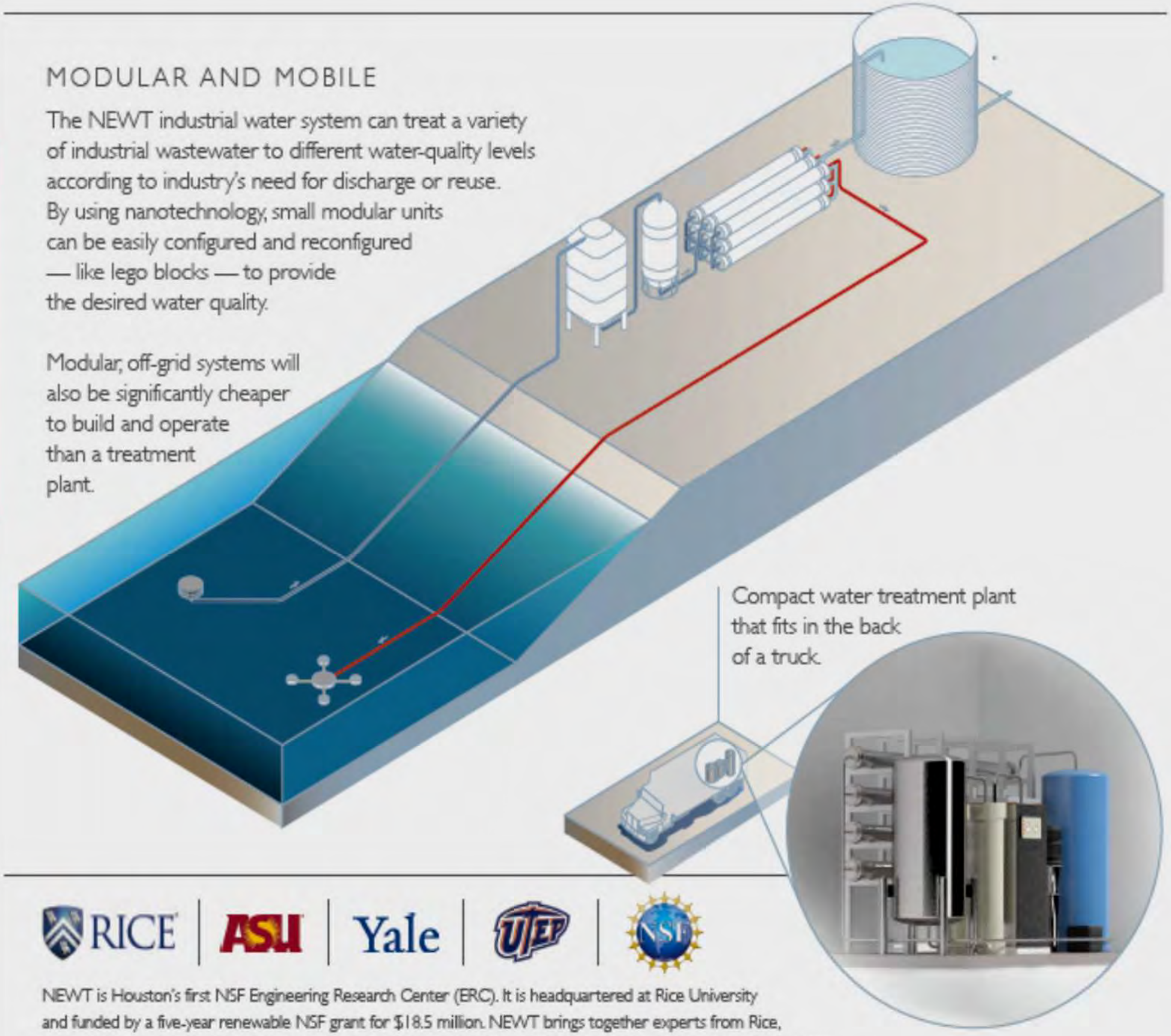
The Nanosystems Engineering Research Center on Nanotechnology Enabled Water Treatment (NEWT) will help provide clean water in a reliable and affordable fashion.

NEWT is developing highly compact, mobile and modular water treatment systems that will be easy to deploy, capable of tapping unconventional water sources, and will enable access to clean water and wastewater reuse almost anywhere in the world.

MODULAR AND MOBILE

The NEWT industrial water system can treat a variety of industrial wastewater to different water-quality levels according to industry's need for discharge or reuse. By using nanotechnology, small modular units can be easily configured and reconfigured — like lego blocks — to provide the desired water quality.

Modular, off-grid systems will also be significantly cheaper to build and operate than a treatment plant.



RICE | ASU | Yale | UTEP | NSF

NEWT is Houston's first NSF Engineering Research Center (ERC). It is headquartered at Rice University and funded by a five-year renewable NSF grant for $18.5 million. NEWT brings together experts from Rice, Arizona State University, Yale University and the University of Texas at El Paso to work with more than 30 partners, including Shell, Baker Hughes, UNESCO, the U.S. Army Corps of Engineers and NASA.

Molecular Dynamics for Optimization

By using computer-aided molecular dynamics simulations, MDM can integrate theory and experimental results to delve deeper into the following topics for various membrane processes:

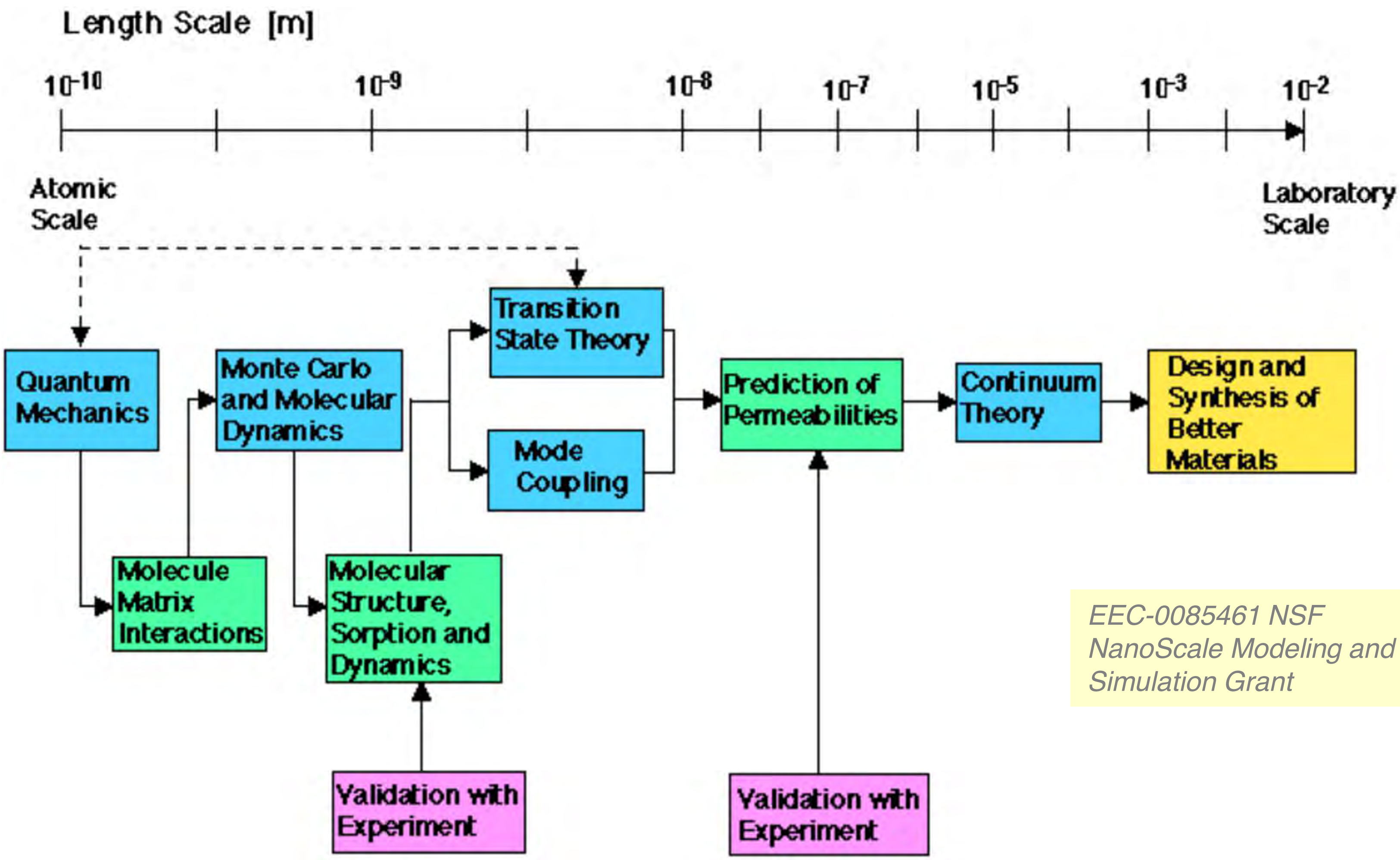
- Studies on transport mechanism
- Fouling investigation

Apart from being applied to well-known water treatment processes such as RO, NF, UF, and MF, MDM can also be used to explore relatively newer technologies, including membrane distillation, forward osmosis (FO) and pressure retarded osmosis (PRO). Areas that can be explored using MDM:

- Membrane distillation: Temperature effects in thermally driven processes.
- Forward osmosis (FO):Characterization of feed and draw solution properties; Comparison of FO performance of polymeric membranes and nanotube membranes.
- Pressure-retarded osmosis (PRO): Interaction of feed and draw solutions with active and porous support layer of membrane and its effects on power generation; Development of PRO membrane.

Molecular Transport in Nanostructured Materials

Computational quantum mechanics will be used as a basis for new and more accurate potential functions, which in turn can be used to produce far more realistic molecular dynamics simulations than are presently possible. The analysis of the trajectories provides short time diffusivities and establishes the transition state geometries. Both results can be extended to macroscopic length scales and to longer times via both generalized hydrodynamics and transition state theory.



EEC-0085461 NSF NanoScale Modeling and Simulation Grant

Challenges in Nanotechnology-based Water Purification Methods

The addition of nanoparticles results in several improvements not only in the membrane properties (hydrophilicity, porosity, permeability, rejection, and membrane structure) but also in the final material properties, which corresponded to thermal, mechanical, and stability enhancements.

However, the following challenges still need to be overcome:

- The possibility of control of the filtration type by using fixed nanoparticle contents represents an important issue in the membrane technology.
- There is not an exact correlation between the final membrane structure and its performance.
- The contributions of each property (hydrophilicity, porosity, and morphology) to the membrane performance are still unclear and need to be elucidated;
- Nanoparticle aggregation in the polymer matrix is often reported by several researchers. Therefore, closer attention needs to be paid to the modification of these particles in order to become them more compatible with the chosen polymer;
- Few studies report the production of the nanocomposite membranes in large scale. Hence, researches should focus this topic.

If the mentioned problems are solved, membrane filtration area can take a huge leap in direction of higher water filtration productivity with a great quality.

Challenges in Nanotechnology-based Water Purification Methods

- Several studies have confirmed that aquaporin-based membranes have higher flux than the normal polymeric membranes thus, the productivity of such membrane has been enhanced in presence of aquaporin.
- However, the production cost of aquaporins are expensive thus fabrication of membrane with such type of material is very expensive in real practice which is another limitation for large-scale production.
- Similarly, biologically inspired membrane, i.e., aligned nanotubes and isoporous block–copolymer membranes have shown enhanced productivity. Not only the productivity is increased for the biologically inspired membrane but also those materials have enhanced the selectivity with exceptionally narrow-pore distributions, which is clearly compressible with any type of normal membrane.
- Biologically inspired membranes have the greatest separation performance than any other membrane, however, their cost and robustness are not established yet, therefore commercialization of such membranes is very challenging indeed.
- Zeolite-based TFN membranes offer moderate performance enhancement and appear nearest to commercial viability.

Open Research Issues

- Research is needed before full-scale operation of nanotechnology for treating natural and wastewaters can be achieved.
- Studies should be conducted under realistic conditions to assess the efficiency of available nanotechnology to validate the nanomaterial-enabled sensing.
- Measure the long-term efficiency of available technologies, which are conducted on a laboratory scale.
- Commercialization of these technologies is possible only by their long-term performance in the treatment of water and wastewater.
- Adoption of an innovative technology strongly depends on the cost effectiveness and potential risks involved.
- At the moment, the cost of nanomaterials is very high, with few exceptions, such as nano-TiO_2, nano-scale iron oxide, and polymeric nanofibers.
- Cost effectiveness can be achieved by regeneration and reuse of these nanomaterials.

Advances in Nanotechnology-based Water Purification Methods

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Department of Chemical Engineering, AUTh
Chemical Process & Energy Resources Institute, CERTH

FIPSE4 Symposium

Porto Carras, Chalkidiki, Greece, June 23-25, 2018

Nanotechnology-based Water Purification

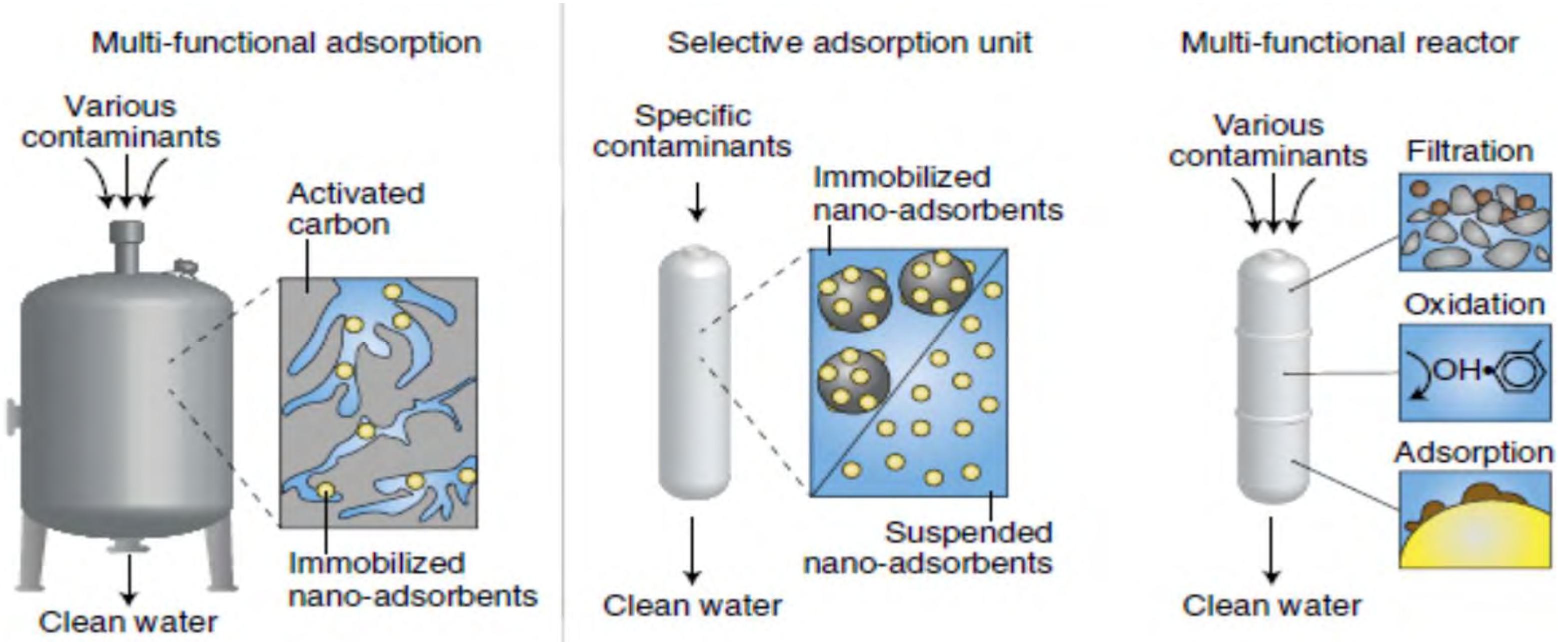
- Introduction
- Water Contaminants
- Conventional Methods & Limitations
- Nanotechnology-Aided Water Purification
  - Nanoadsorbents
  - Membranes
  - Nanophotocatalysts
  - Water Disinfection
  - Commercially Available Devices
- Metrics
- Conclusions

Adsorption Processes

Nanoadsorption Processes

Nanotechnology-based platforms for decontamination processes

- Centralized water treatment applications: Nanoadsorbents can be immobilized in a conventional adsorbent (e.g., activated carbon) and facilitate multifunctional adsorption of organic and inorganic pollutants (left).
- Decentralized applications: Nanoadsorbents can be used to design a selective adsorption system for removing specific contaminants of concern, in either immobilized form or in suspended form with magnetic properties for low-energy separation and recovery. Nanoadsorbents can also be integrated in a small-scale multifunctional treatment system to purify water by several mechanisms such as filtration, oxidation, and adsorption.

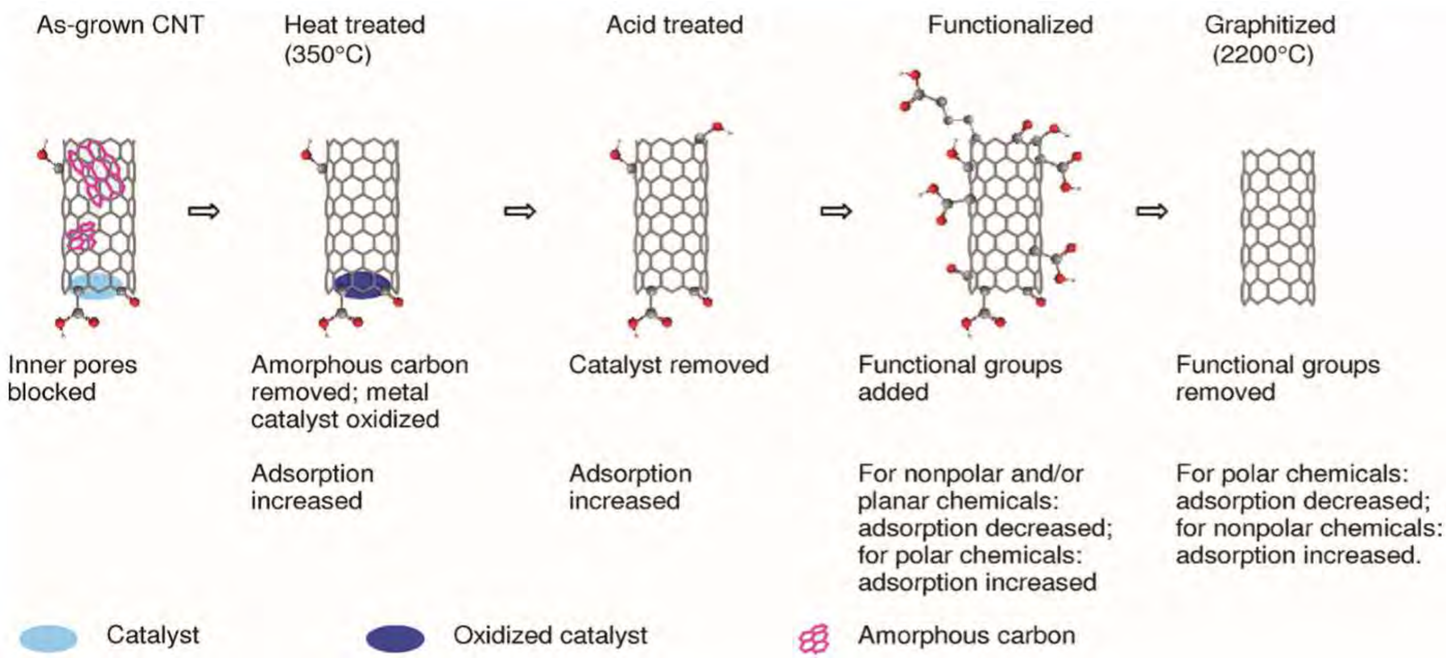


Nanoadsorbents

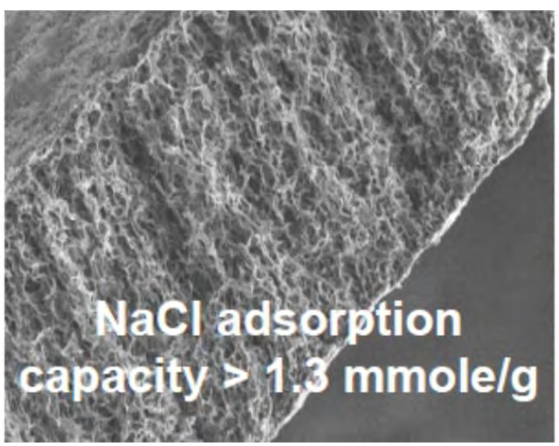
Nanomaterials	Desirable Nanomaterial Properties	Enabled Technologies
• CNT	• High specific surface area, highly assessable adsorption sites, diverse contaminant-CNT interactions, tunable surface chemistry, easy reuse.	• Contaminant preconcentration / detection, adsorption of recalcitrant contaminants.
• Nanoscale metal oxide	• High specific surface area, short intraparticle diffusion distance, more adsorption sites, compressible without significant surface area reduction, easy reuse, some are superparamagnetic.	• Adsorptive media filters, slurry reactors.
• Nanofibers with core–shell structure	• Tailored shell surface chemistry for selective adsorption, reactive core for degradation, short internal diffusion distance.	• Reactive nanoadsorbents
• Nanocomposites	• Immobilized, synergistic effects of both materials.	• Nanoadsorbents, selective adsorbents
• Nano modified Biochar	• High surface area, sustainably produced from agricultural/ environmental residues, can house a variety of nanoparticles to target contaminants.	• Adsorption media filters

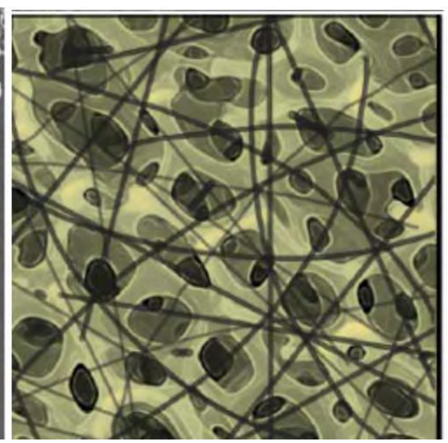
Carbon Nanotubes

Adsorption properties affected by CNT functional groups

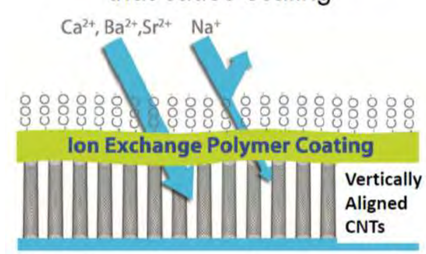


Nano-Enabled CDI for Scaling Control applying CNTs





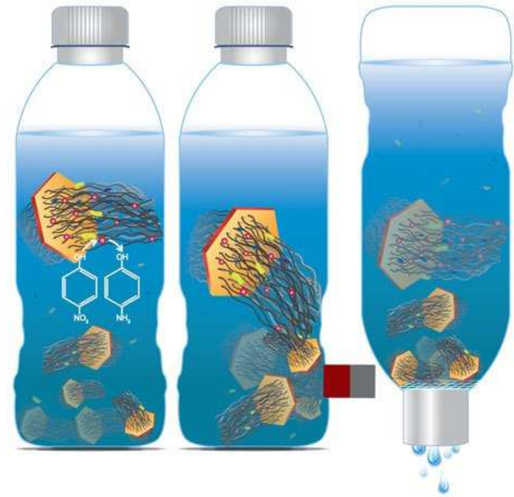
IX polymers enable preferential removal of divalent cations that cause scaling



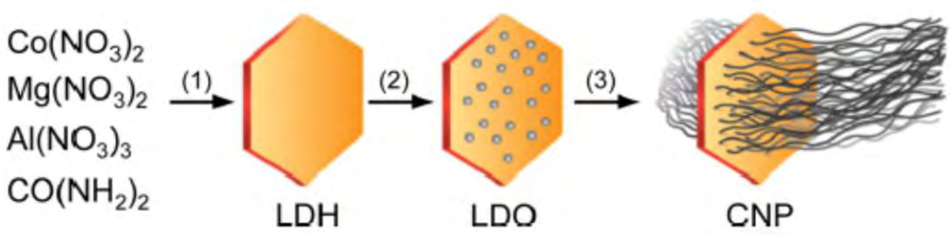
CNTs/graphene enhance sorption capacity, kinetics, mechanical strength and electrical conductivity.

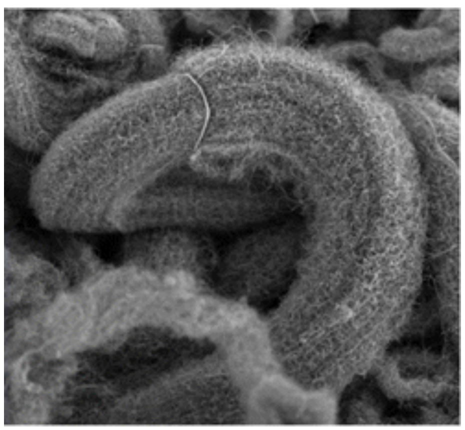
Carbon Nanotube Ponytails

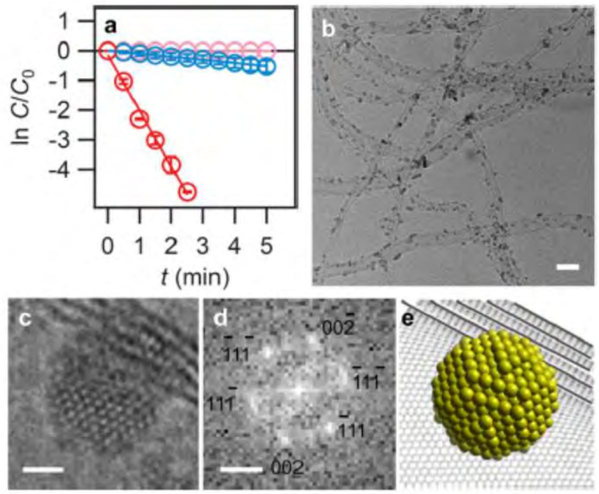
- The direct use of unbounded CNTs, poses health risks to humans and ecosystems because they are difficult to separate from treated water.
- The synthesis of carbon nanotube ponytails (CNPs) via integration of CNTs into micrometer-sized colloidal particles, greatly improves the effectiveness of post-treatment separation using gravitational sedimentation, magnetic attraction, and membrane filtration.



Synthesis of CNPs



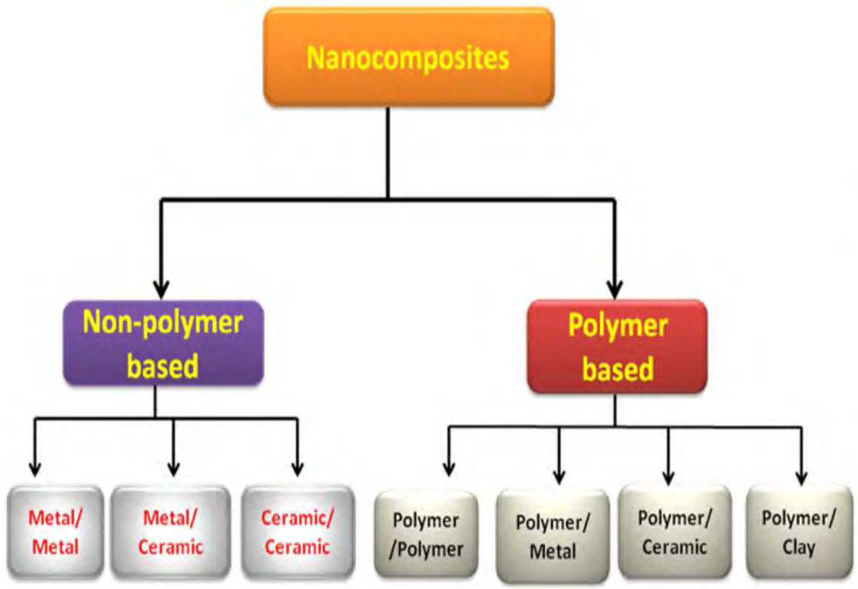




Wang et al., 2014

Catalytic reduction of p-nitrophenol (PNP) by CNPs and enhancement of catalytic performance with decoration of Pd NPs

Nanocomposites

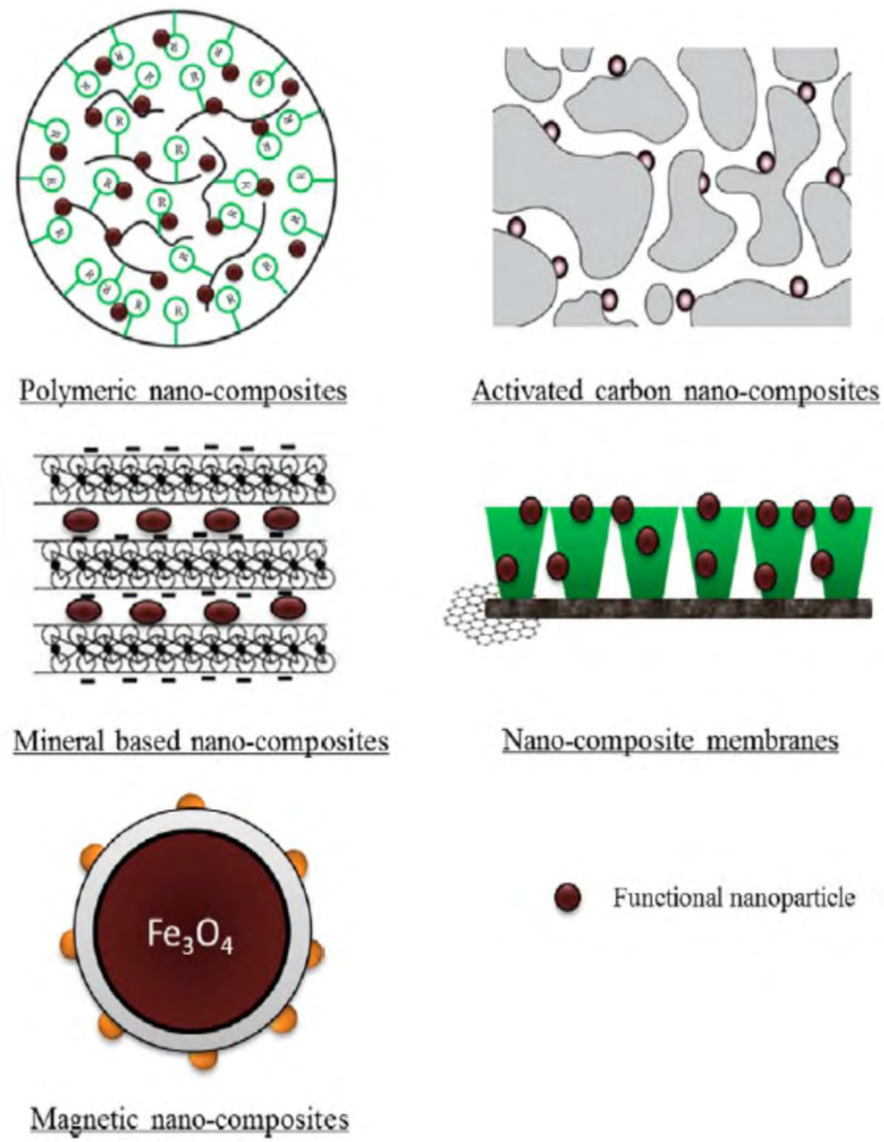


Properties

- Surface complexation
- Electro-static attraction
- π–π bonding
- Hydrogen bonding
- Hydrophobic effect
- Inhibited e-/h+ recombination
- Reduced band gap energy
- Cell membrane disruption
- Signal enhancement

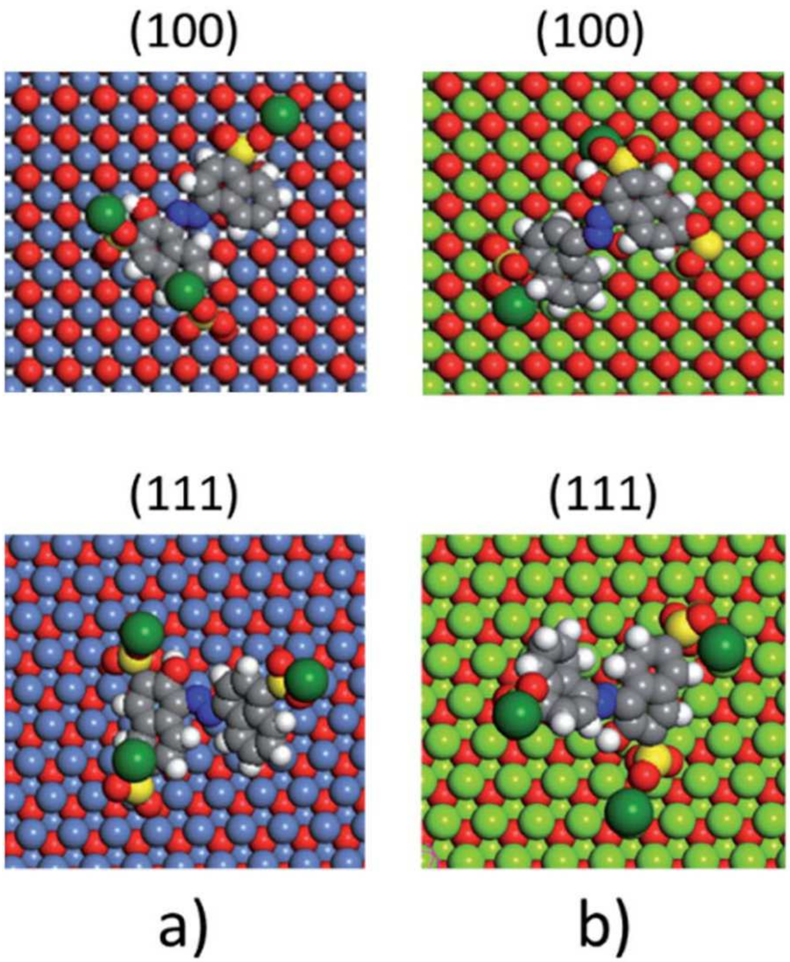
Functions

- Adsorption/separation
- Reduction/oxidation
- (Photo)catalysis
- Anti-bacterial
- Sensing



Molecular Dynamics for Optimization

Computational modeling studies on silica-embedded NiO/MgO nanoparticles for adsorptive removal of organic pollutants from wastewater

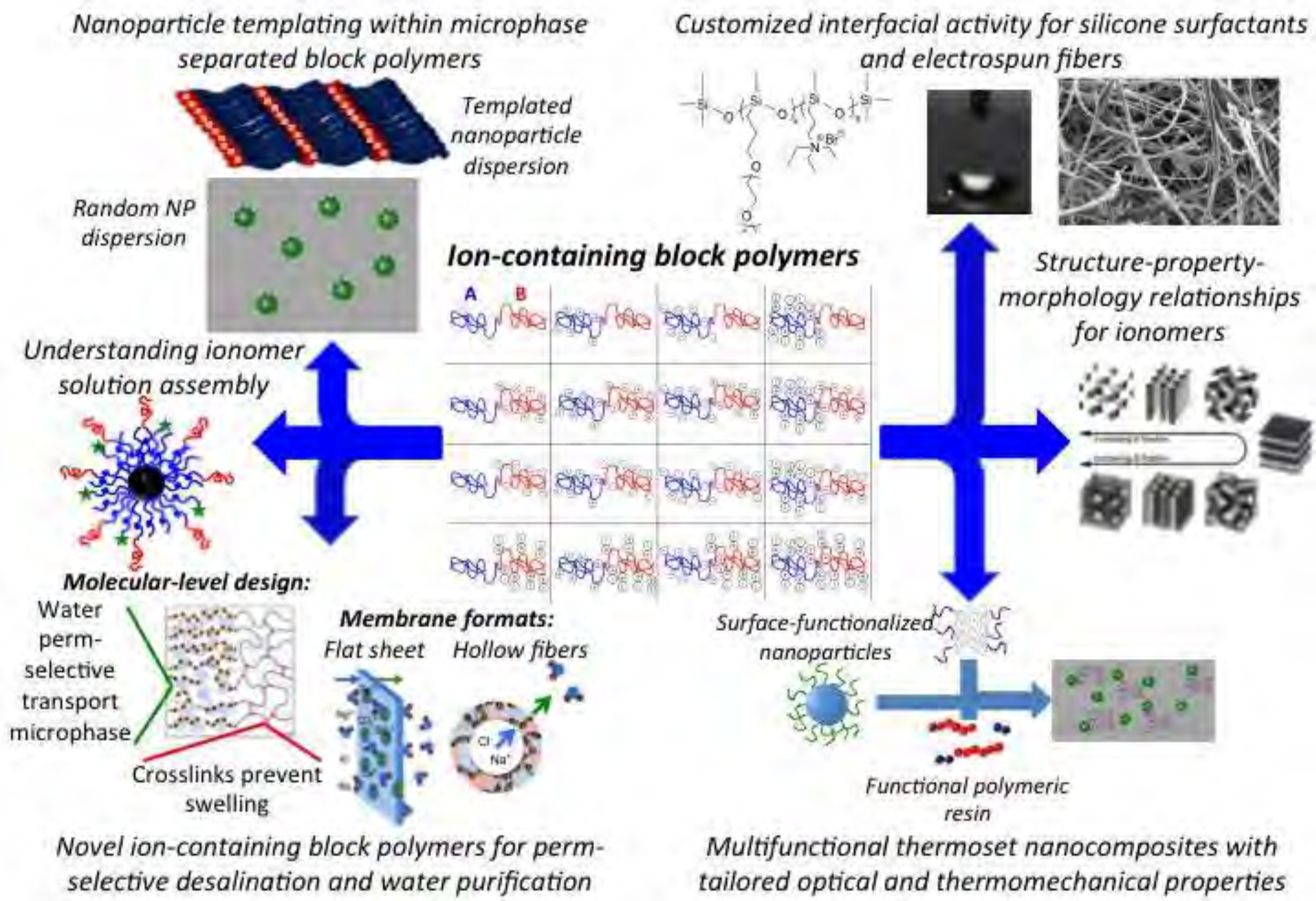


- Computational modeling and DFT calculations of the interaction between the model molecules and the surfaces of the prepared nanoparticles were carried out to get more mechanistic insights into their adsorptive behaviors.

CPK representation of the adsorbed AR27 molecule onto the (100) and (111) surfaces of: (a) NiO and (b) MgO. Grey atoms represent carbon, bright blue atoms represent nitrogen, white atoms represent hydrogen, yellow atoms represent sulfur, dark green atoms represent sodium, pale green atoms represent chlorine, bright green atoms represent magnesium, pale blue atoms represent nickel, dark yellow atoms represent silicon and red atoms represent oxygen.

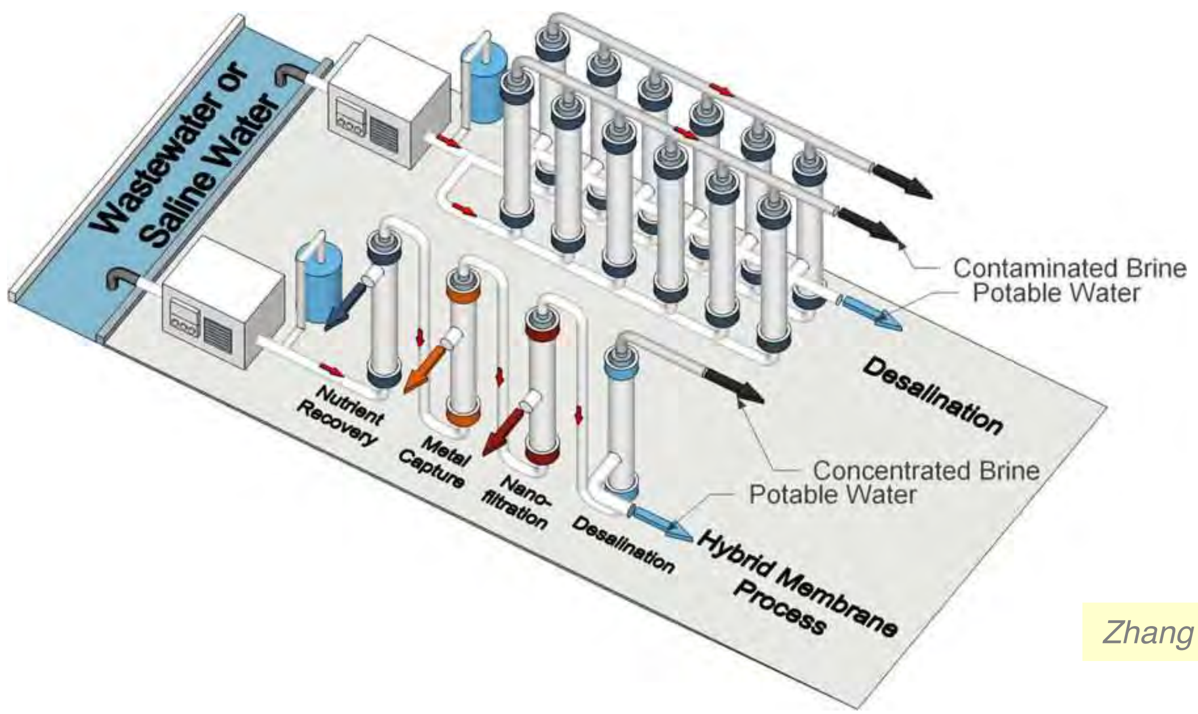
El-Qanni et al., 2017

Polymer-based Nanocomposites



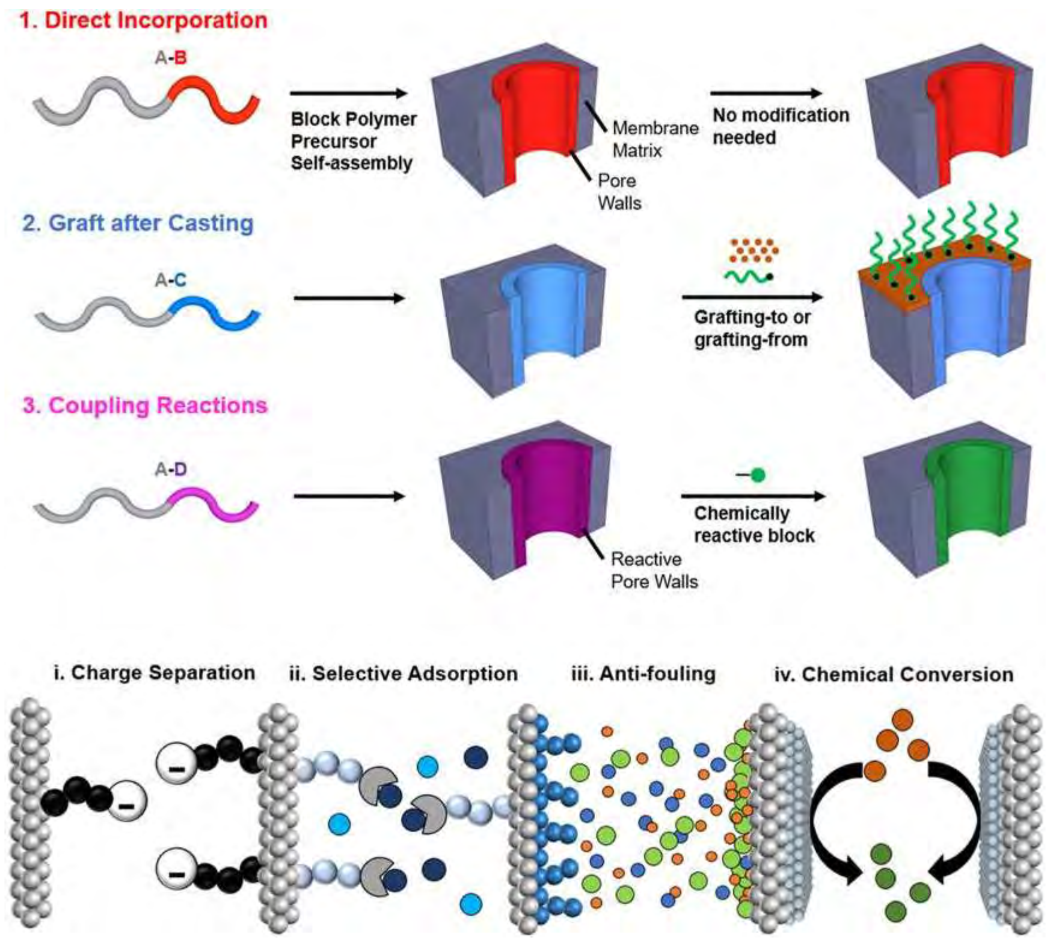
Molecular Dynamics for Optimization

- A conceptual process flow diagram for water treatment by a desalination process and a hybrid membrane process.
- The hybrid membrane process is designed with a cascade of separations that target the generation of product water at the purity required for the end applications as well as the recovery of valuable resources.
- In this type of process, resource recovery and selective solute removal can be achieved by membranes with functional pore wall chemistries, as represented by each module, that are integrated in series.
- Self-assembled block polymer membranes have great potential for implementation in desalination and hybrid membrane processes due to their well-defined nanostructure and nearly-limitless surface chemistries.



Zhang et al., 2018

Molecular Dynamics for Optimization



An illustration of the broad range of potential applications where membranes with functional pore wall chemistries could be utilized

(1) The functional chemistry (red block) can be incorporated into the precursor block polymer prior to membrane fabrication. With the identification of suitable SNIPS parameters, a self-assembled membrane with functional pore walls that require no further functionalization reactions is generated.

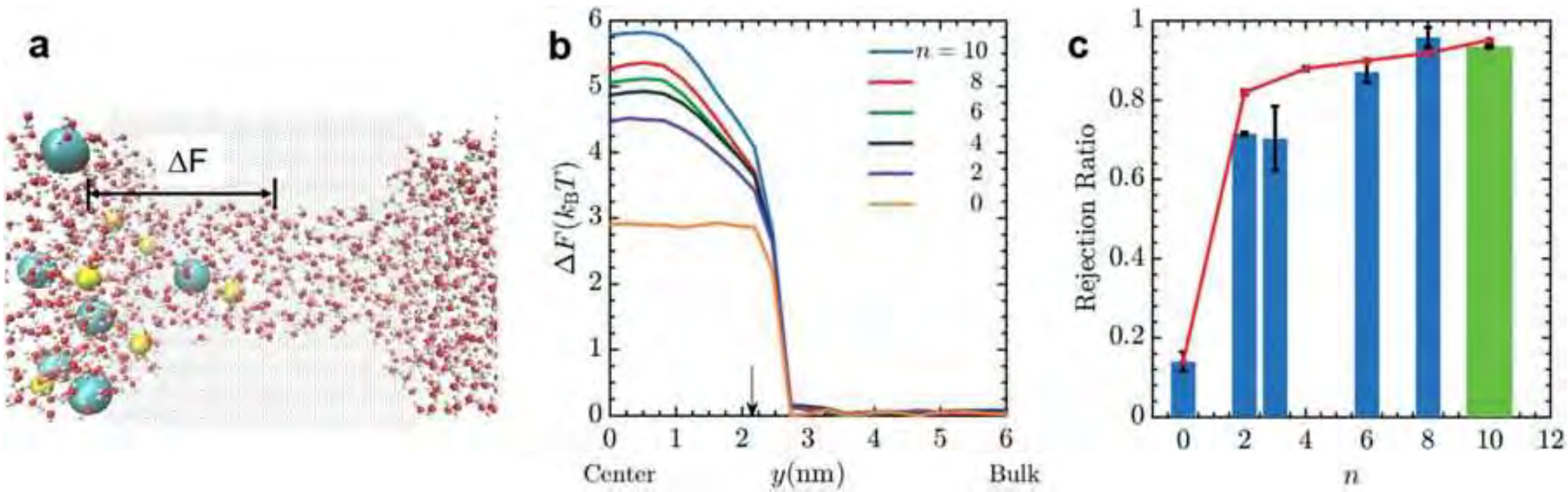
(2) The block polymer chemistry facilitates formation of a self-assembled structure. Subsequently, the surface of the membrane is modified using a coating (orange dots) to which functional chemistries are attached (green brushes).

(3) The pore wall-lining block (magenta) is designed as a reactive chemistry that can be converted to a variety of functional chemistries through coupling reactions that are consistent with roll-to-roll processes.

Zhang et al., 2018

Molecular Dynamics for Optimization

Molecular scale information that guides the systematic design of pore wall chemistry can be determined through carefully constructed MD simulations

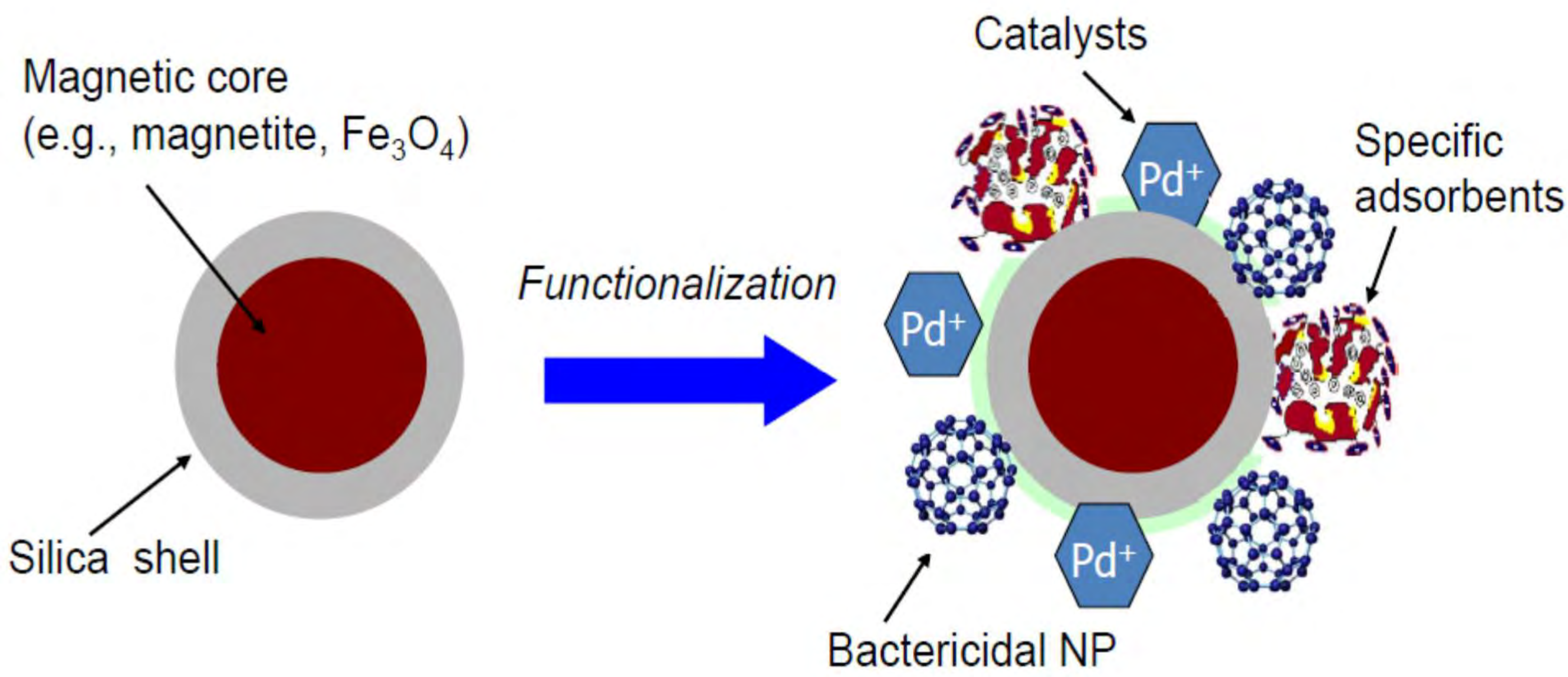


a Schematic showing the measurement of the free energy change of ions (blue and yellow) as they are entering the pore (atoms forming the membrane are gray).
b The PMF profiles for the translation of a magnesium cation from a bulk solution into the pore of a membrane. The entrance of the functionalized pore is indicated by the arrow at ~2 nm. The orange line represents a parent membrane, n = 0; the other lines correspond to simulations executed with increasing spacer arm lengths. The spacer arm length, n, is defined as the number of carbon atoms between the pore wall linkage and the terminal charged functional group.
c Simulated and experimental rejection for magnesium cations plotted as a function of spacer arm length, n. The simulation results, which were calculated using the free energy barrier obtained from b, are shown with the red line. The experimental data, which are represented by the bar graphs, were measured using a 10 mM MgCl2 feed solution.

Zhang et al., 2018

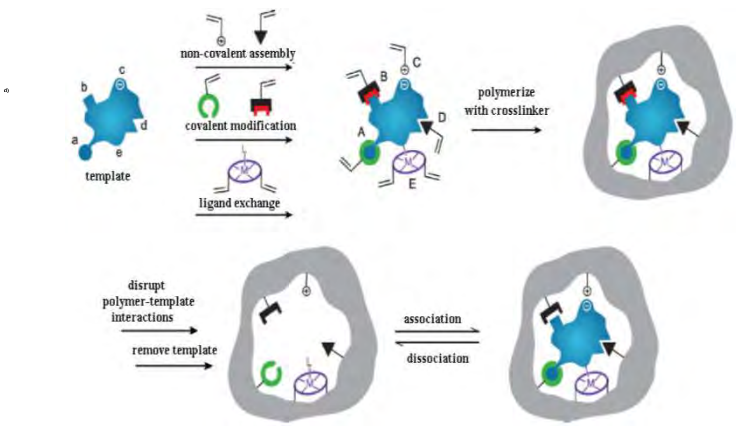
Multifunctional Nanocomposites

- Selective removal of target contaminants by functionalized NPs supported in macroscale structures or subject to magnetic separation for enhanced removal kinetics and easier reuse.

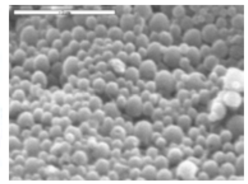


Molecular Imprinting Technology

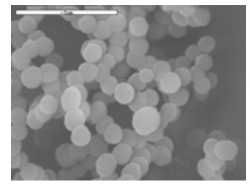
➤ Molecular imprinting is a strategy used for introducing regions of highly specific molecular arrangements into a polymeric matrix.



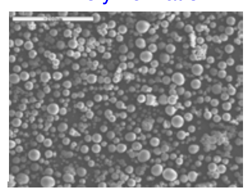
✓Mini-emulsion Polymerization



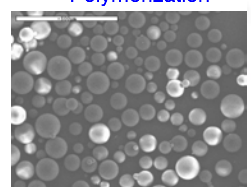
✓Precipitation Polymerization

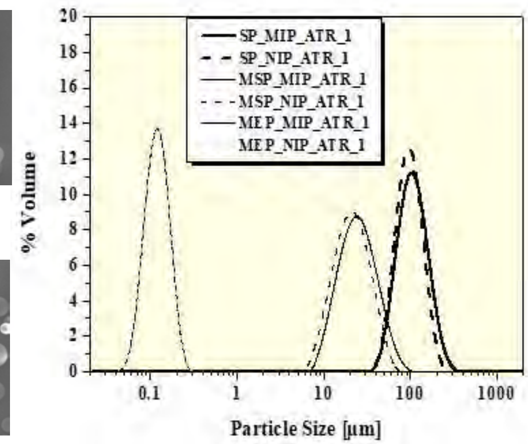


✓Micro-suspension Polymerization



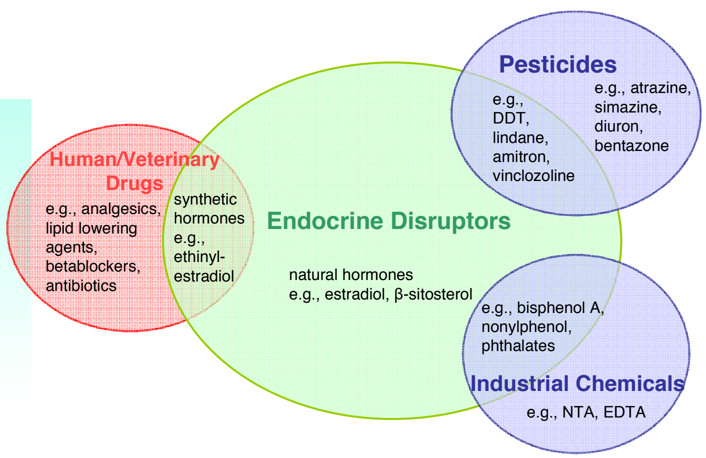
✓Suspension Polymerization



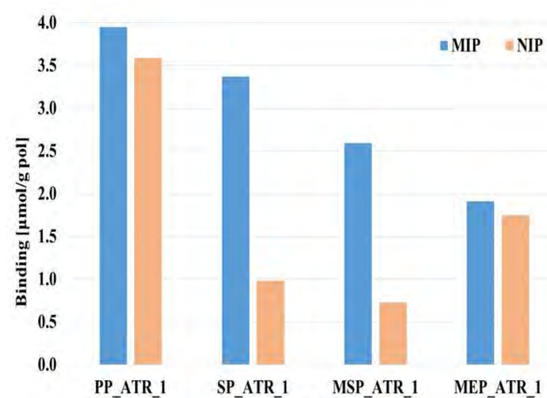


Application Areas

- Analytical Separations
- Bioseparation
- Clinical Analysis
- Diagnostics
- Drug Delivery Systems
- MIPs Films for Sensors
- Removal of SOCs from Water

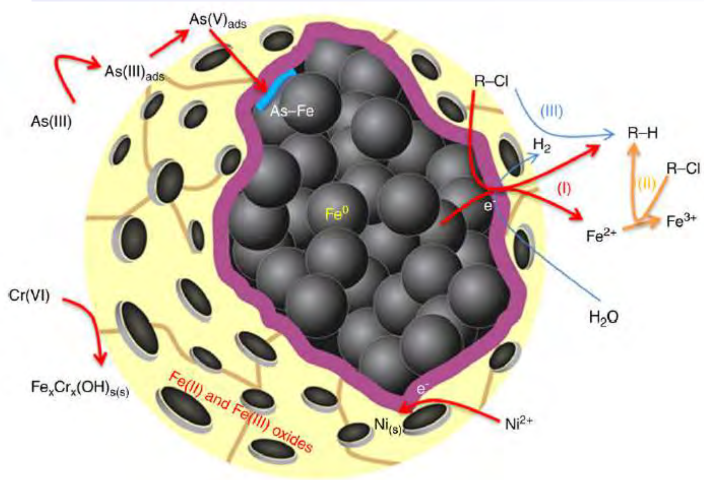


Target Compounds

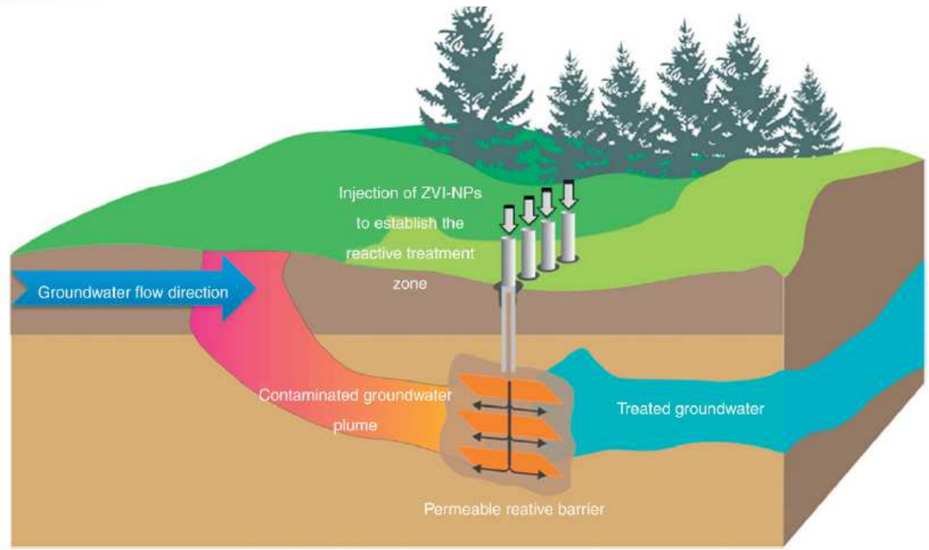


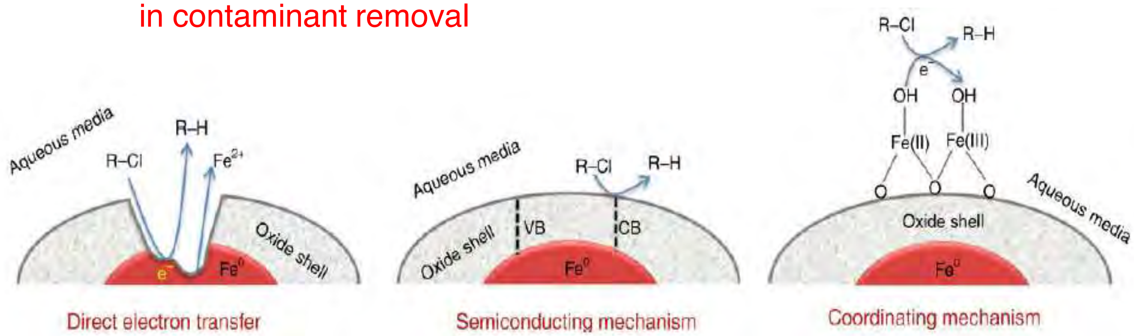
Zero-Valent Iron Nanoparticles

- ✓ ZVI-NPs possess higher reactivity and higher surface area than ZVI. Moreover, the unique capabilities including sufficient mobility within porous media and sufficient reactive durability provide high interest for both in situ and ex situ applications in remediation of contaminated groundwater.
- ✓ In the removal of chlorinated organics, ZVI-NPs act as a potent and cost-effective electron donor from the iron surface to chlorinated hydrocarbons.



Core–shell structure of ZVI-NPs and its role in contaminant removal





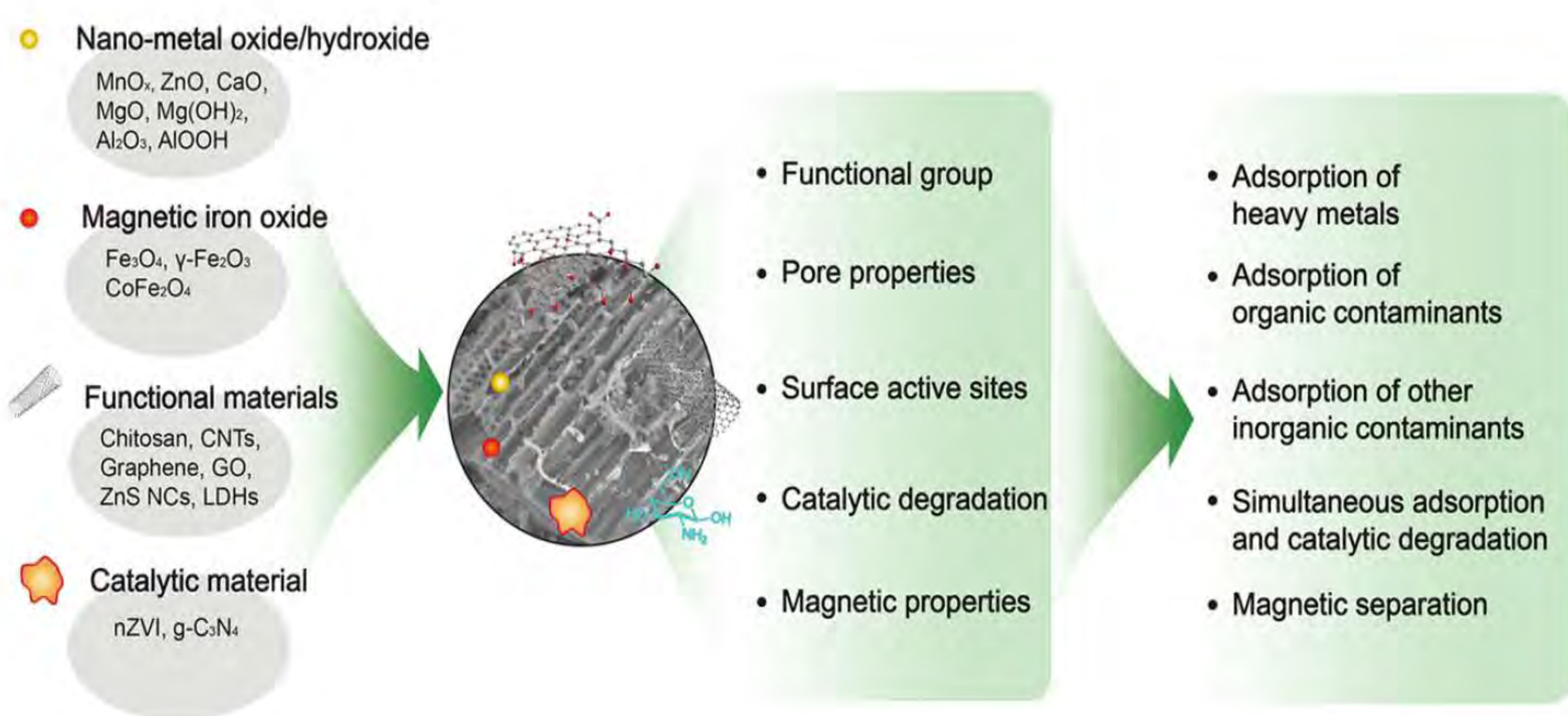
Removal mechanism of chlorinated hydrocarbons by ZVI-NPs

Permeable reactive barrier utilizing ZVI-NPs injection technology for treating contaminated zones

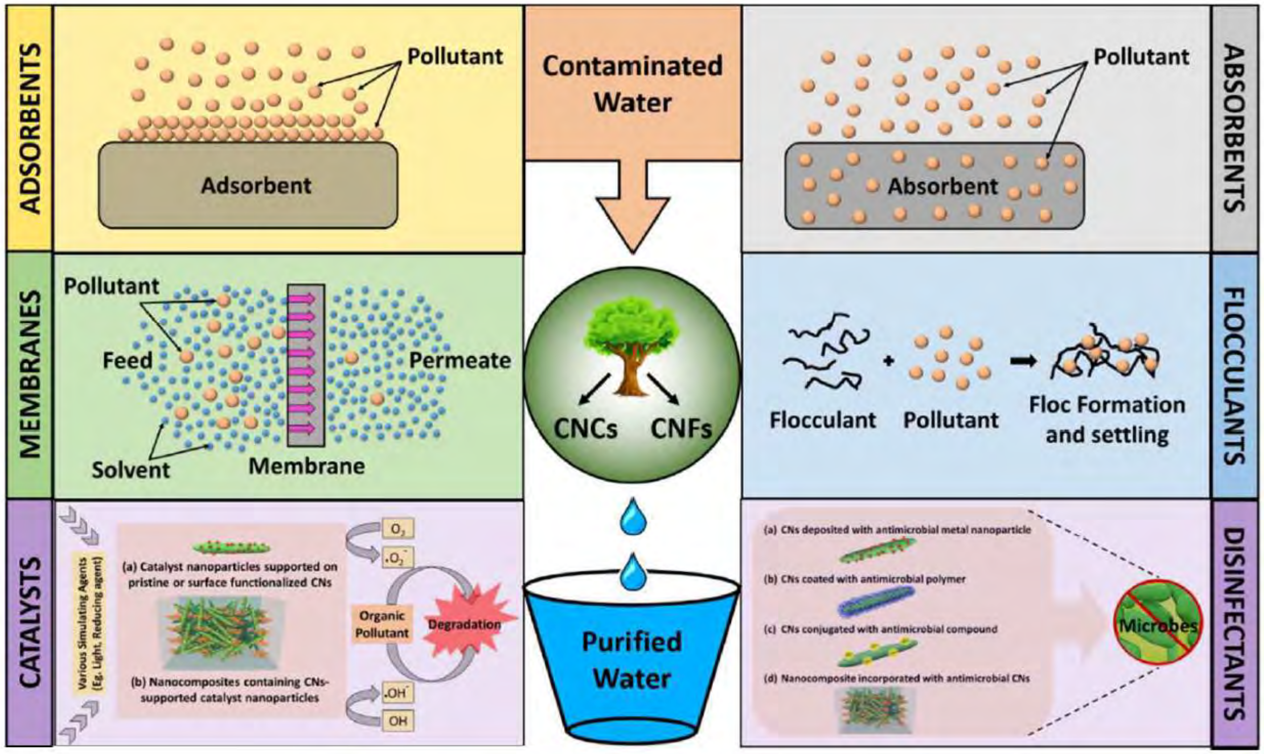
Chapter 4, Water Purification, 2017

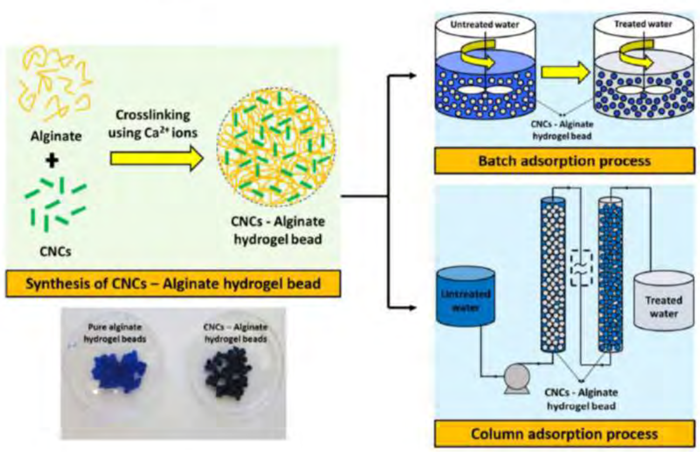
Biochar

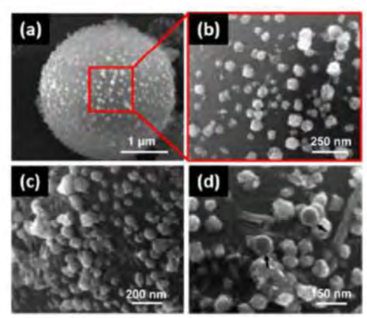
- Biochar is a carbon-rich solid derived by pyrolyzing biomass with little or no oxygen.
- Biochar-based nanocomposites combine the advantages of biochar with nano-materials, thus exhibiting improved functional groups, pore properties, surface active sites, catalytic degradation, and easy separation.
- Catalytic material-coated biochar can exert simultaneous adsorption and catalytic degradation function for organic contaminants removal.

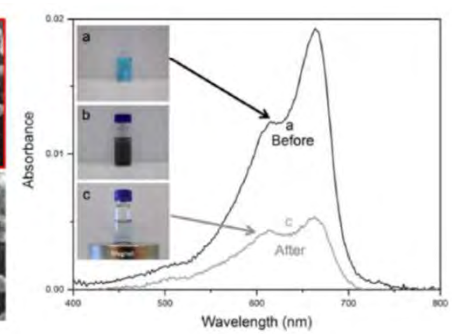


Nanocellulose based Nanocomposites



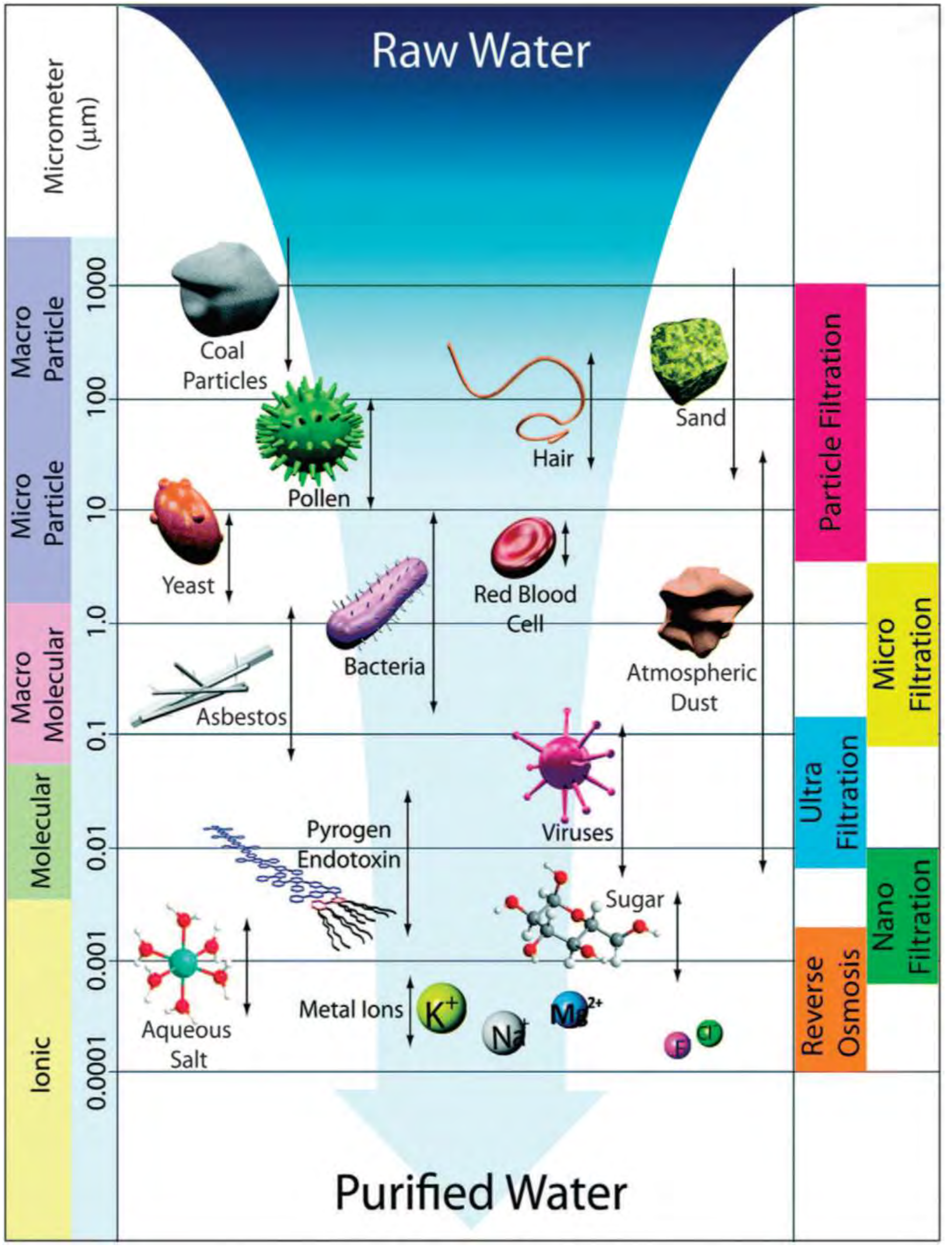






Membranes

Membranes



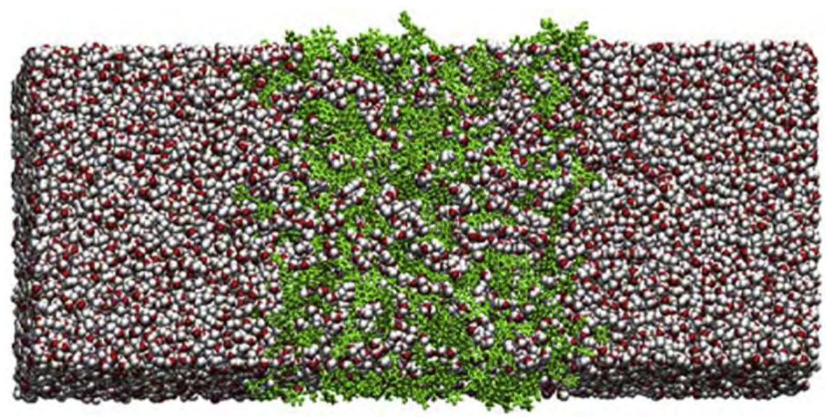
- Nanoengineered surfaces can reduce fouling, biofilm formation, and scaling, effectively reducing efficiency losses and improving component lifetimes in the technologies that employ heated fluids.
- Improvements over current membrane technologies that would also be beneficial for alternatives to RO that utilize membranes, such as forward osmosis and membrane distillation.
- Nanotechnology-enabled working fluids have also the potential to boost heat-carrying capacity, which would be advantageous for technologies that employ heat exchange (e.g., membrane distillation).

Molecular Dynamics for Optimization

- A thorough investigation of membranes as well as their transport and material properties is a key to understanding the governing principles and unresolved issues of membrane processes.
- Through molecular dynamics (MD) simulations, static and dynamic properties of membrane separation systems may be investigated on a molecular level.
- Two approaches in MD are important in investigations about membrane-based water treatment processes: the equilibrium and non-equilibrium molecular dynamics (NEMD) simulations.

Using both of these approaches in investigations would produce in-depth analyses of the behavior of microscopic channels.

- ✓ For equilibrium conditions, there should be no difference in chemical potential between two solution
- ✓ Reservoirs separated by a channel. On the other hand, for a non-equilibrium simulation, they applied a fixed force on a layer of water molecules having a defined length to obtain a hydrostatic pressure difference.



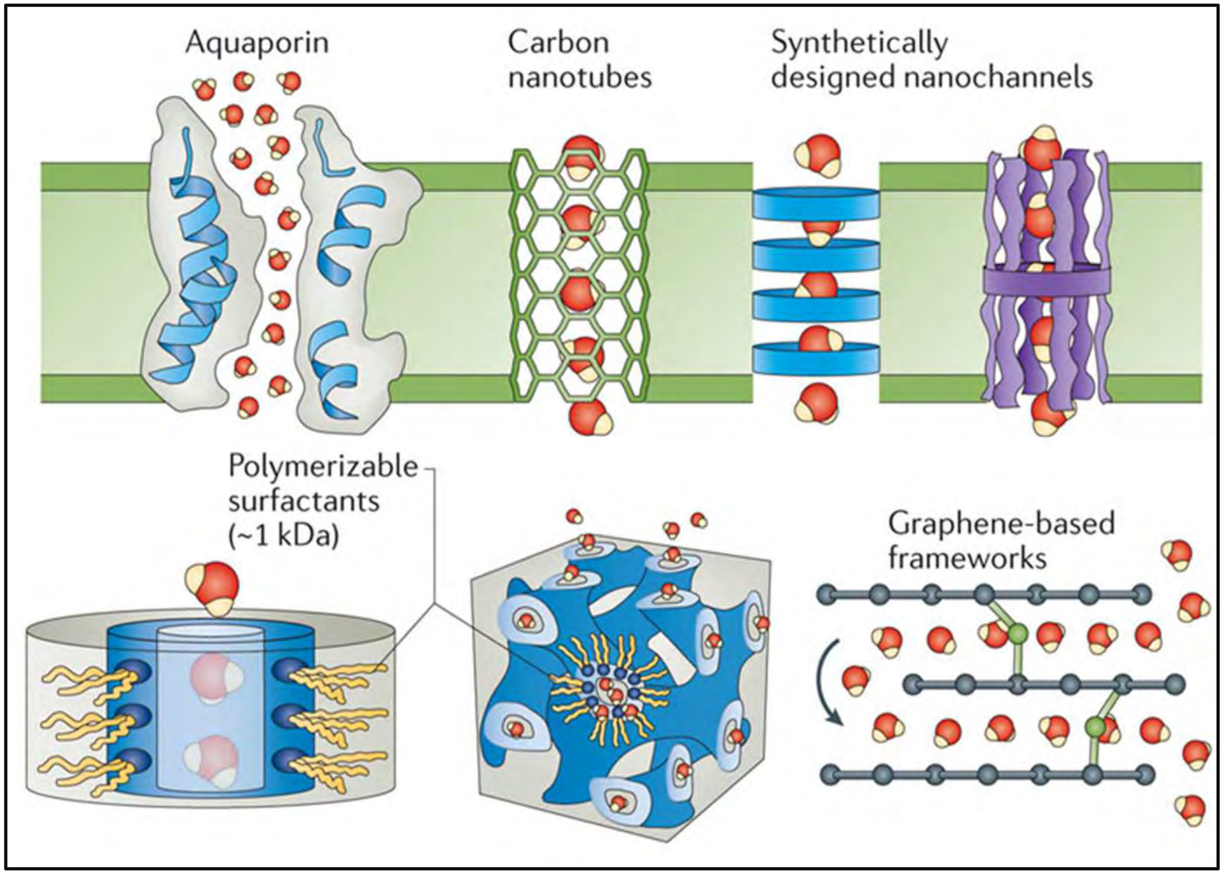
Configuration of water-solvated polymer membrane after equilibration. Particle representation: water (red and white, VdW model) and polymer membrane (green, licorice model).

Ebro et al., 2013

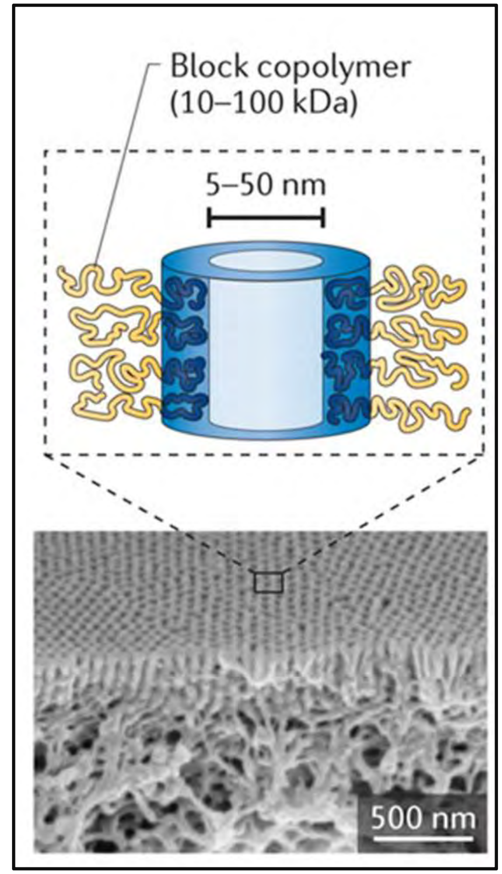
Recent Trends in Membrane Synthesis

➢ Selective membranes formed using molecular-level design.

Sub-nanoporous membranes

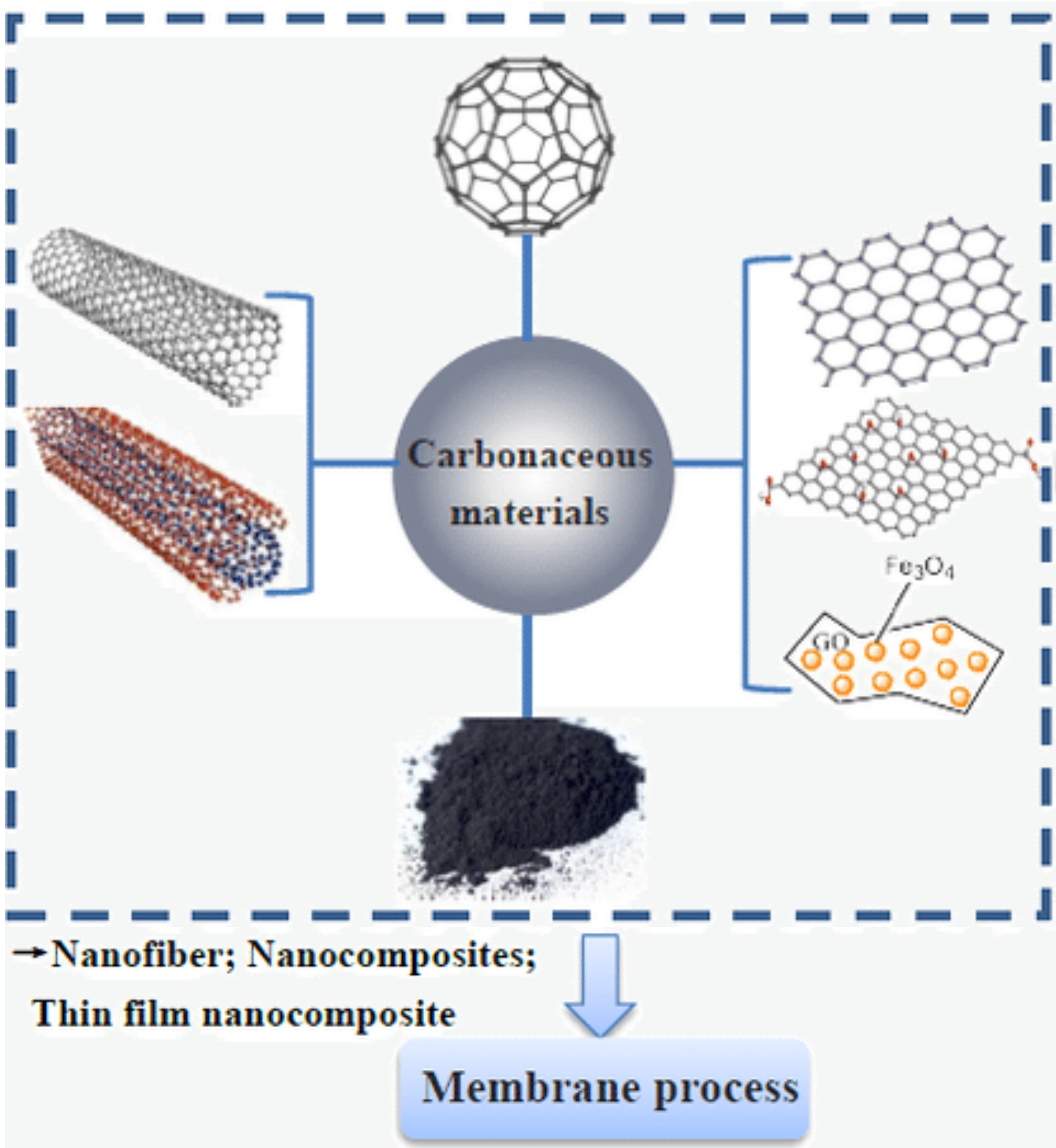


Isoporous membranes

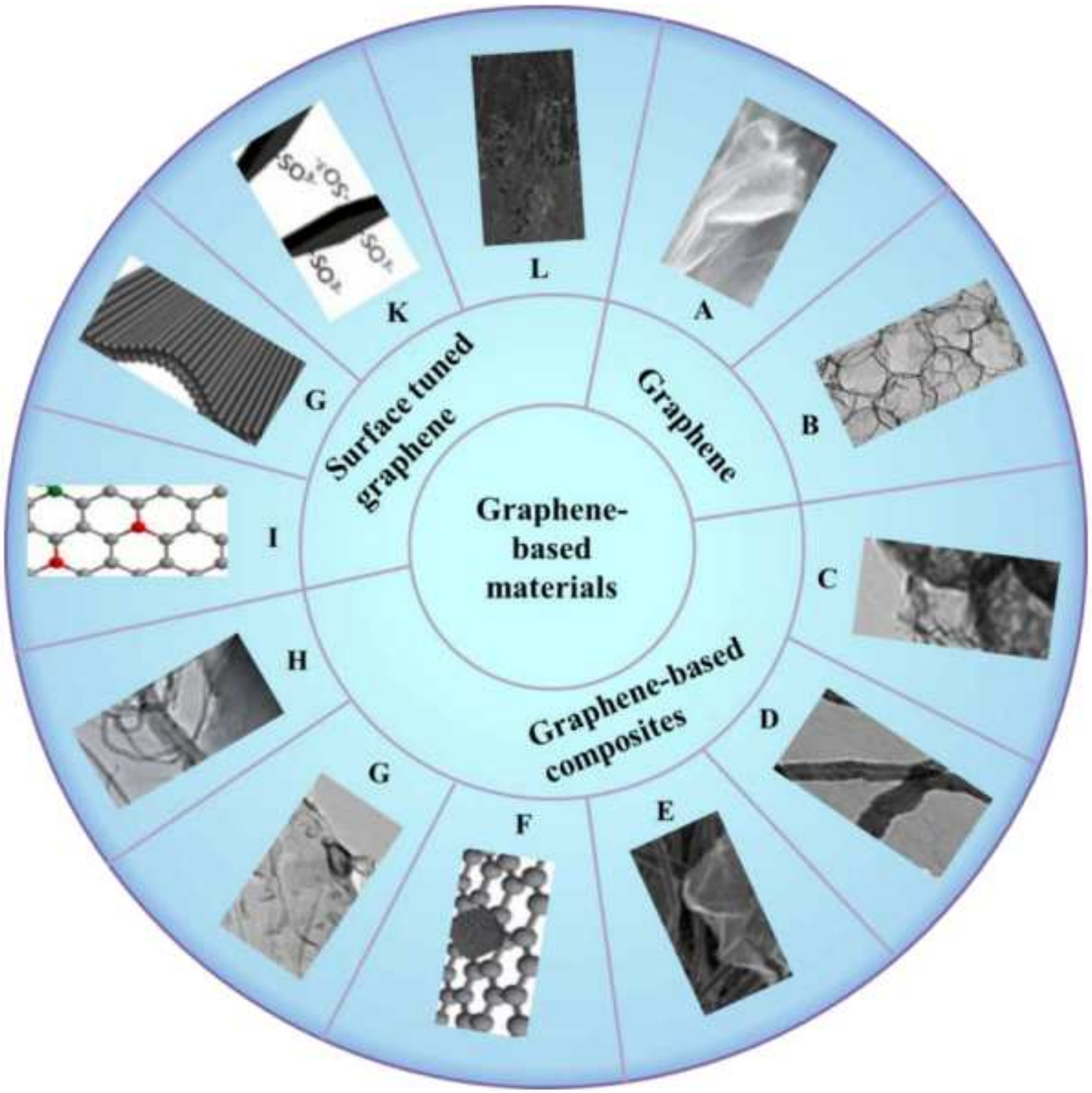


Elimelech, M. et al. (2016)

Carbon-based Nanomaterials



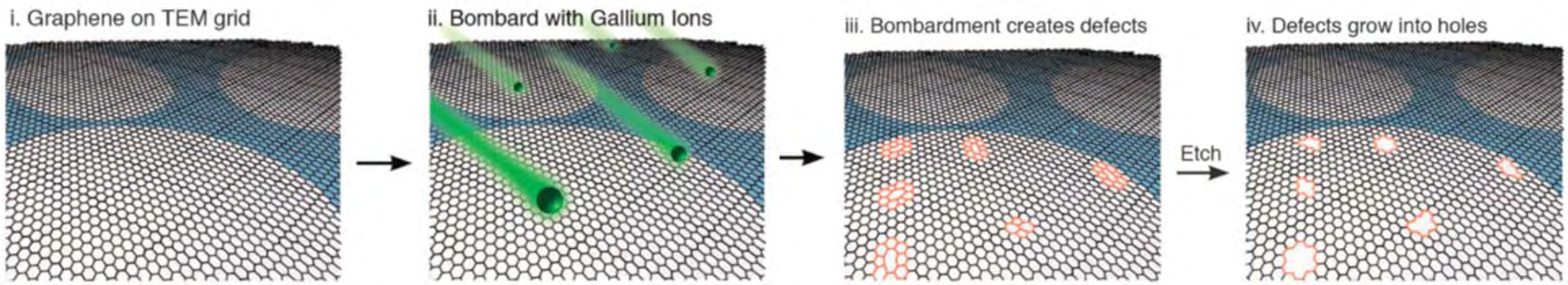
Graphenes



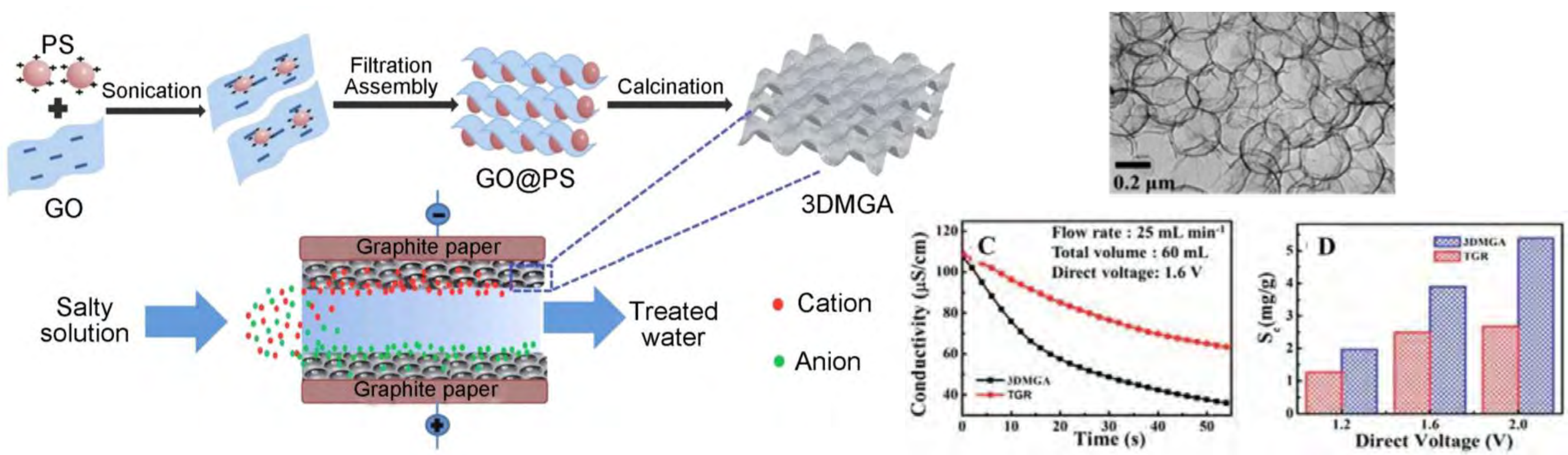
(A) Graphene nanosheets
(B) Porous graphene
(C) Graphene-porous carbon composites
(D) Graphene-carbon nanotube composites
(E) Graphene-activated carbon nanofibers composites
(F) Graphene-metal oxide composites
(G) Graphene-polymer composites
(H) Multi-component graphene-based composites
(I) Nitrogen-doped graphene
(J) Nitrogen-doped Graphene based composites
(K) Functionalized graphene
(L) Functionalized graphene based composites

Graphenes for Separation Processes

- ✓ Process for the inclusion of controlled pores in a monolayer graphene membrane by ion bombardment followed by chemical oxidation



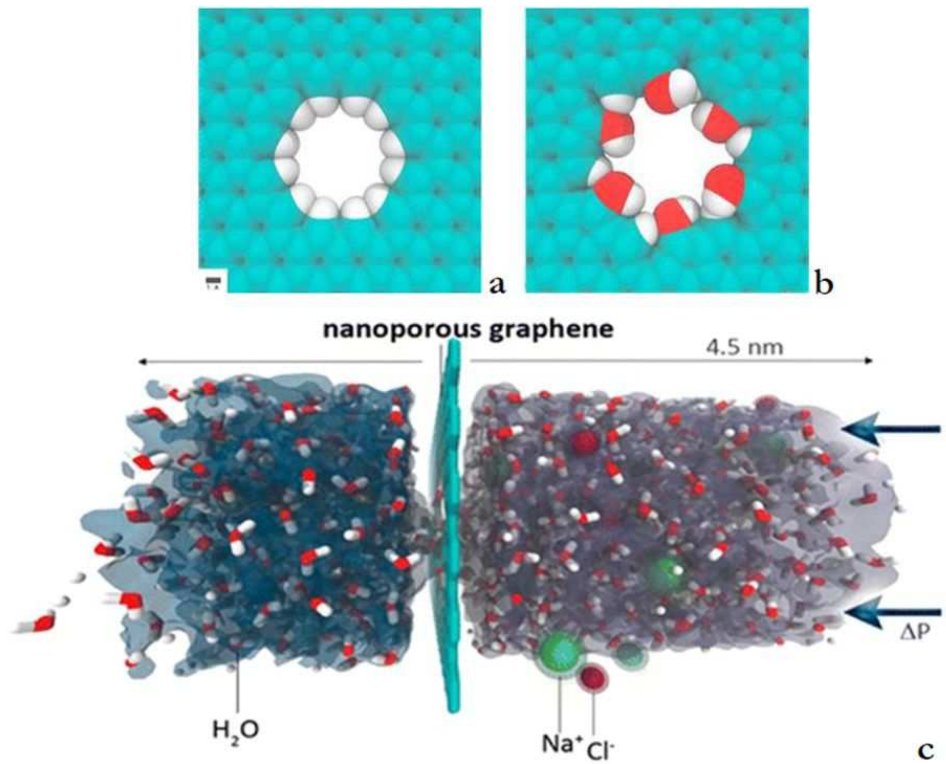
- ✓ 3D macroporous graphene architectures by a simple template-directed method, using polystyrene microspheres as sacrificial templates, are designed to prevent the aggregation and restacking of graphene sheets.



Molecular Dynamics for Desalination

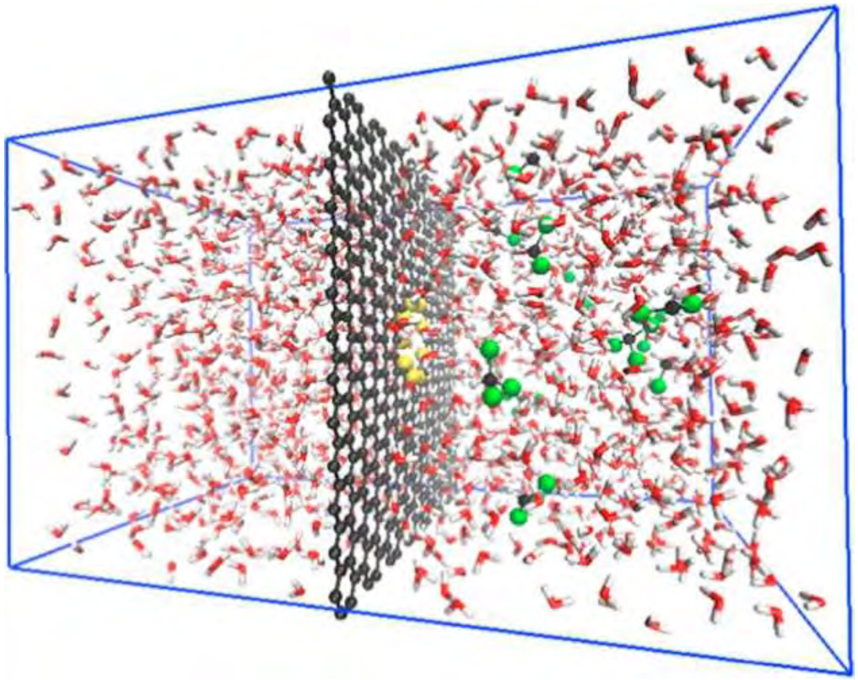
- The simplest graphene-based desalination membrane can be produced by making nanoscale pores in a layer of graphene. This results in a flexible, chemically and mechanically stable separation membrane, based on a single-atomic layer thick material with target use in desalination.

Water can penetrate subnanometer size pores, while salt ions larger than water molecules cannot and because of the ultralow thickness of the membrane, NPG was predicted to have greater water permeability coefficients than current thin-film composite RO membranes.
Complete salt rejection was predicted to be possible for hydroxylated pores of diameter 0.45 nm.
Such performances were achieved for a 5 μm diameter sample of NPG.
The material was obtained by oxygen plasma etching of graphene grown through chemical vapor deposition (CVD).
Scaling up of NPG membranes is extremely challenging, because it requires the formation of a large area of a single-layer, defect-free, graphene, and the scalable formation of uniformly sized nanopores.



Molecular Dynamics for Purification

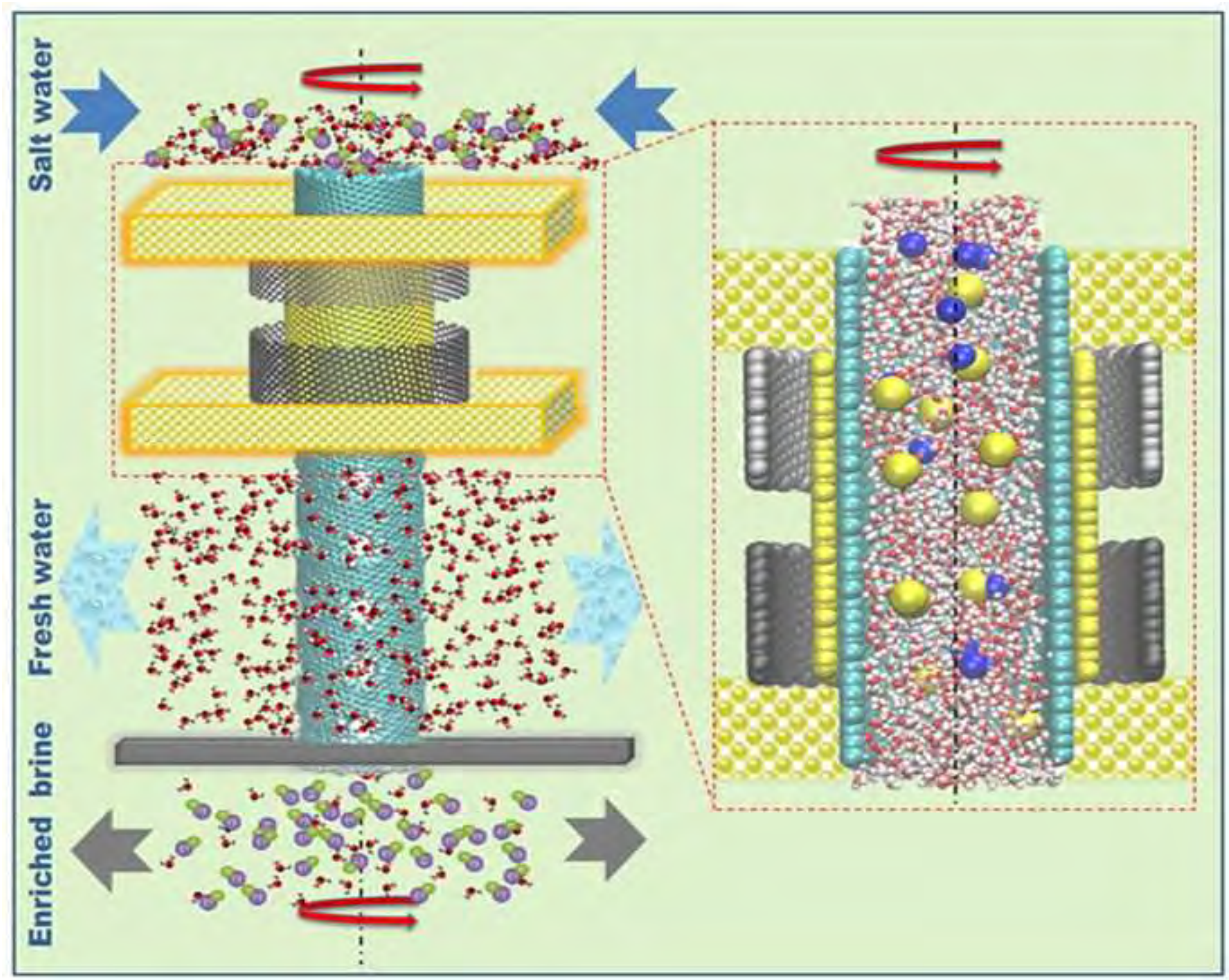
- Molecular dynamics simulations of trihalomethanes (THMs) separation from water were performed using a functionalized nanoporous graphene under induced pressure.



The simulated system included a functionalized graphene immersed in an aqueous solution of THMs. External pressure was applied to the system along the z axis of the functionalized nanoporous graphene. F-pore and H-pore terminated graphenes of different sizes were used.
The results showed that a functionalized nanoporous graphene with a small diameter was impermeable to THMs.
In contrast, a functionalized nanoporous graphene with a large diameter was shown to be permeable to THMs.
The permeation of THMs and water molecules across the functionalized graphene was dependent on the chemical function of the pores, the size of pores, and the pressure.
A snapshot of the simulated system containing graphene membrane for THMs separation; (green: chlorine, black: carbon, yellow: fluorine, red: oxygen and white: hydrogen).

CNT Membrane Filters

Design concept of rotating CNT membrane filter and the desalination mechanism based on the working principle of the double wall rotating CNT

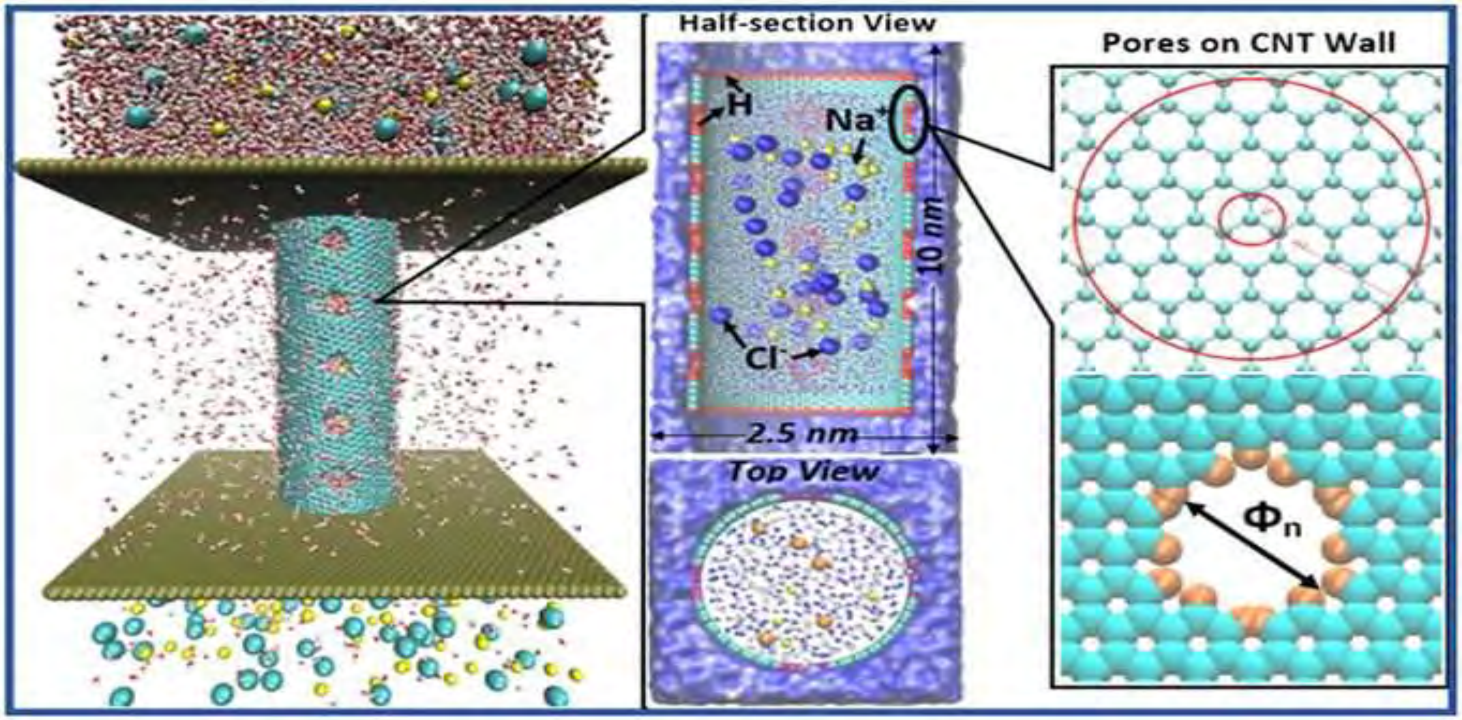


Tu et al., Nature Scientific Reports, 2016

CNT Membrane Filters

Configuration and working principle of RCNT-MF device

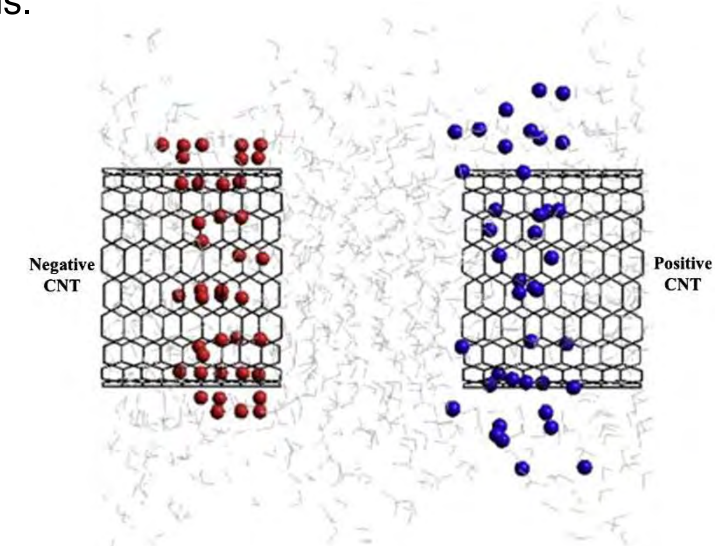
Tu et al., Nature Scientific Reports, 2016

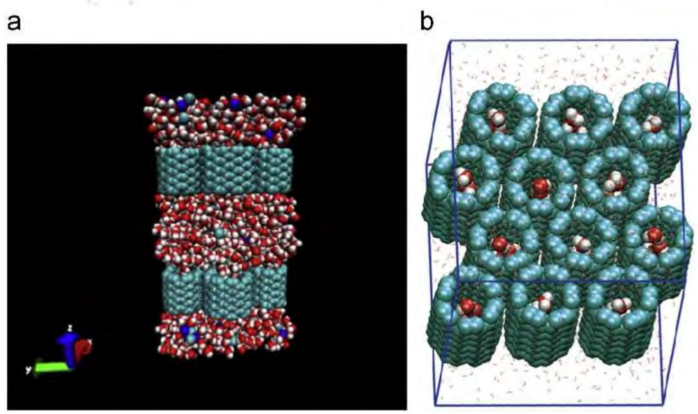


- ✓ There is a CNT motor at the top of the proposed desalination device, which provides power to keep the CNT filter rotating.
- ✓ The functional part of RCNT-MF is a partial double-wall CNT system, and when electric voltage is applied to the outer CNT it may exert a torque to the inner CNT. This may be done by properly choosing chiral vectors for the outer and the inner CNTs so that the outer wall may conduct electricity while the inner wall cannot.
- ✓ For the desalination purpose, holes (d<1 nm) are formed on the wall of the inner CNT, via ion bombardment or the e-beam lithography.
- ✓ For the chiral type CNTs, the rotating motion will generate a negative pressure that draws the salt water into the top entrance of the RCNT-MF.

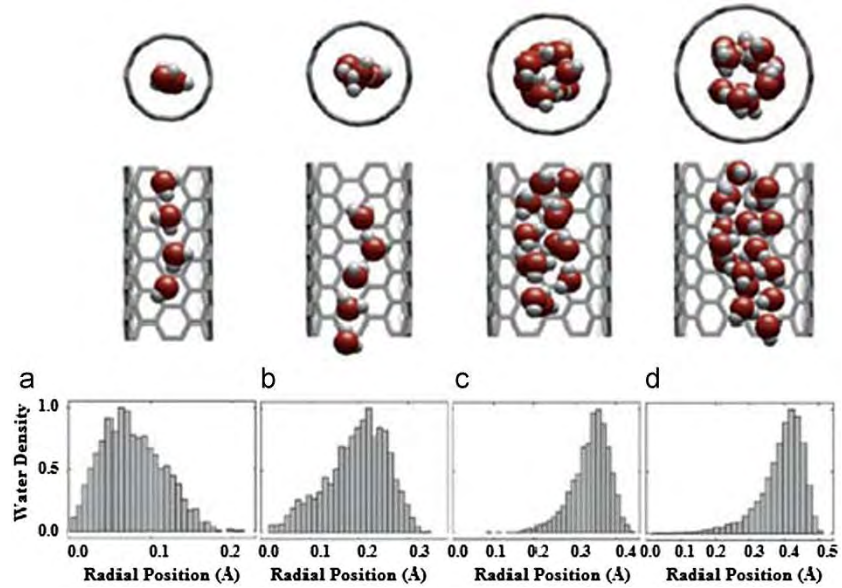
Molecular Dynamics for Optimization

Snapshot taken after finishing a 2-ns simulation of ion separation using charged carbon nanotubes. The blue spheres represent the chloride ions while the red ones are the sodium ions.





Structure (top) and radial density distribution (bottom) of water inside four different armchair-type boron nitride nanotubes having (n,n) chirality: (a) (5,5), (b) (6,6), (c) (7,7), and (d) (8,8).

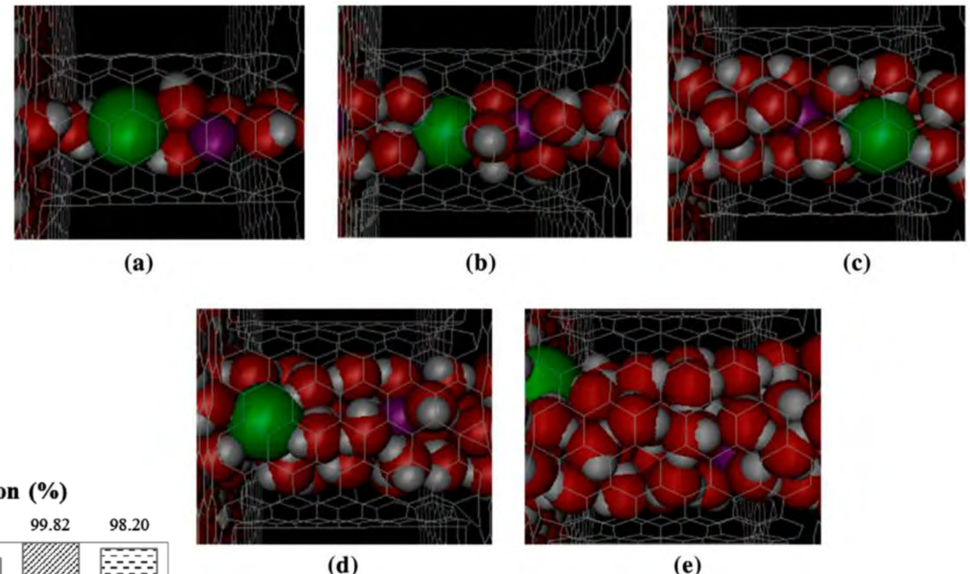


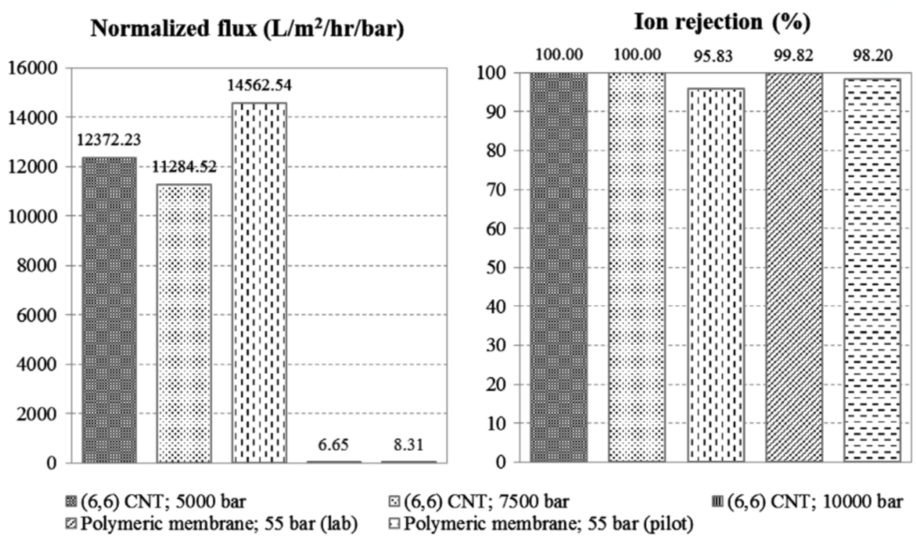
(a) Setup for the simulation of forward osmosis (FO) desalination. Low-concentration (at the center) and high concentration (at both ends, connected by periodic boundary conditions) NaCl solution chambers are separated by two sets of CNT layers.

Molecular Dynamics for Optimization

Molecular dynamics simulation of seawater reverse osmosis desalination using carbon nanotube membranes

Snapshots of ion permeation during different simulations used to visualize the typical coordination numbers of sodium (purple) and chlorine (green) ions with hydrating water molecules (red/white) inside the CNT pore: (a) (6, 6) CNT, 25000 bar, (b) (7, 7) CNT 7500 bar, (c) (8, 8) CNT, 7500 bar, (d) (9, 9) CNT, 7500 bar, and (e) (10, 10) CNT, 7500 bar.





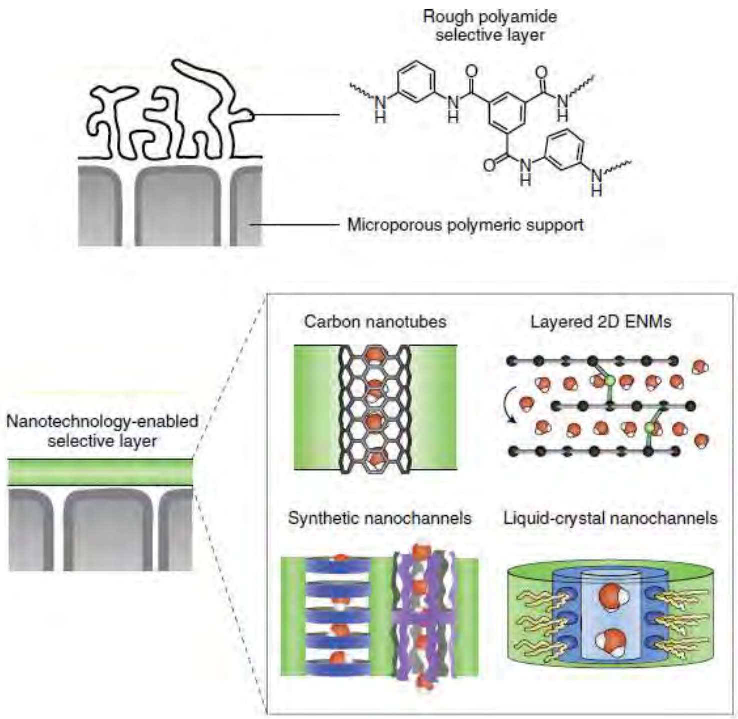
Comparison of ion rejection, normalized flux, and price per effective membrane area of (6, 6) CNT membrane and conventional polymeric membranes.

Mi Kim., 2016

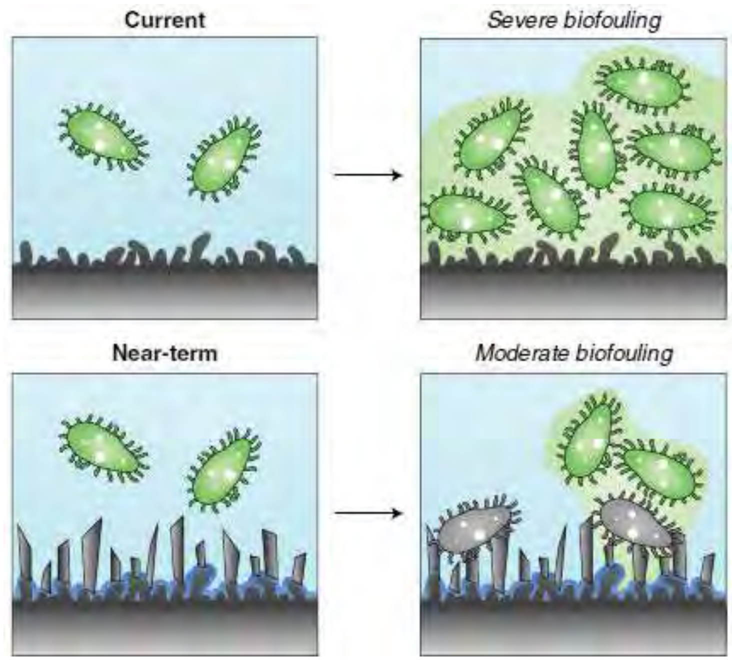
Nanotechnology-enabled RO for desalination

- Desalination membranes used in high-membrane-area spiral-wound modules.

- Current polymeric and potential nanotechnology-enabled desalination membranes.



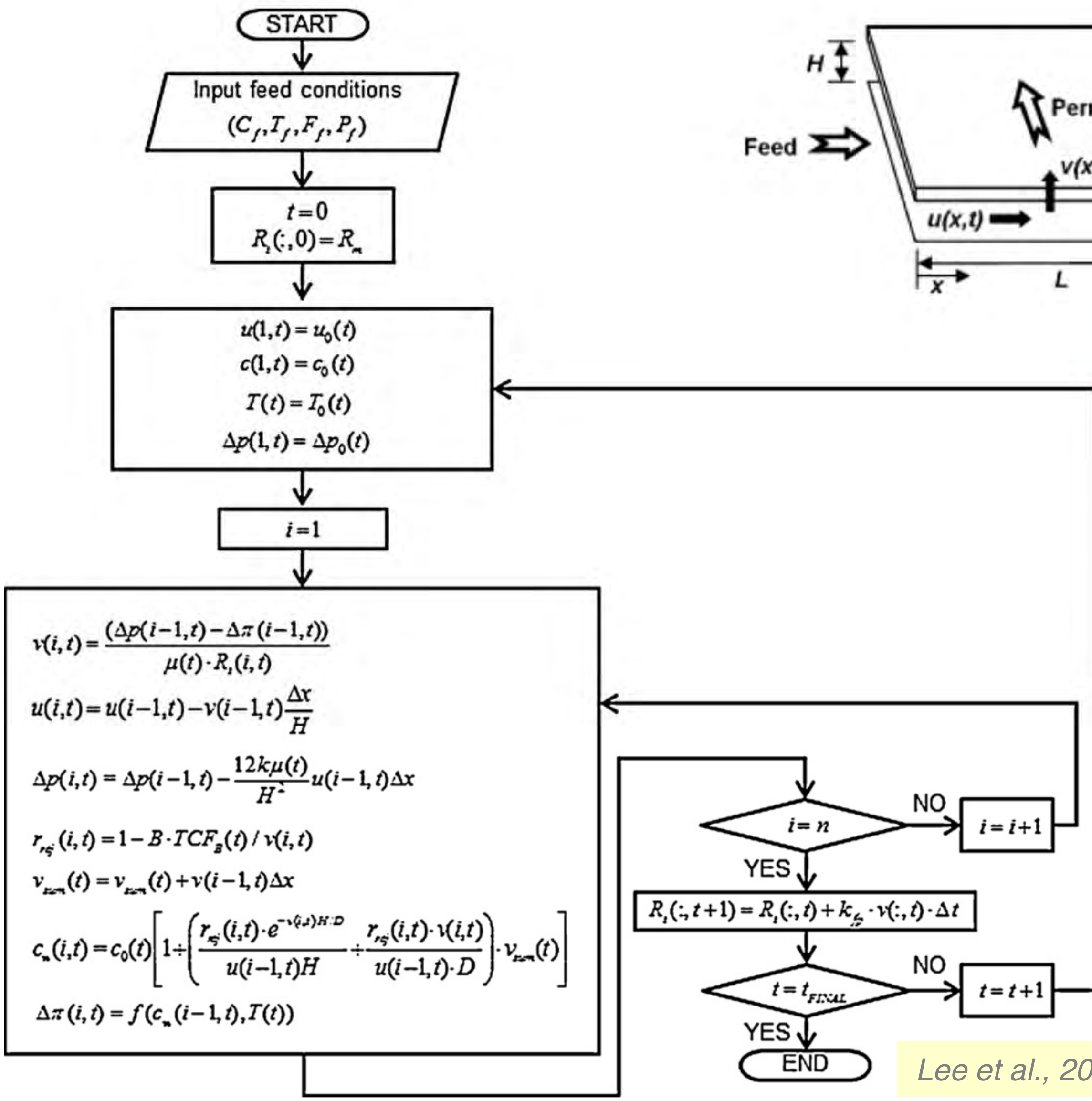
- Use of nanotechnology to combat biofouling

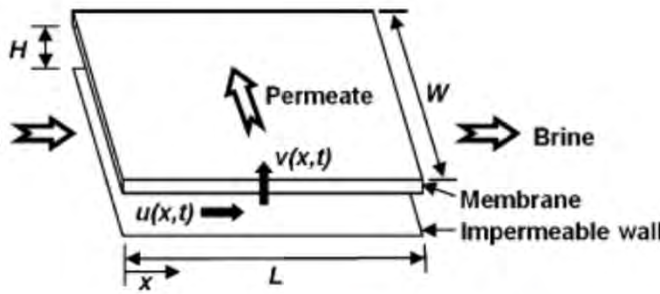


✓ Biofouling can be partially mitigated in the near-term using anti-adhesive coatings (dark blue) and surface-attached ENMs that enable contact-mediated bacterial inactivation (grey shards).

Process Optimization

A fouling model for simulating long-term performance of sea water RO desalination process





Lee et al., 2012

- A model considering time-variant fouling and concentration polarization has been developed to simulate the long-term membrane performance.

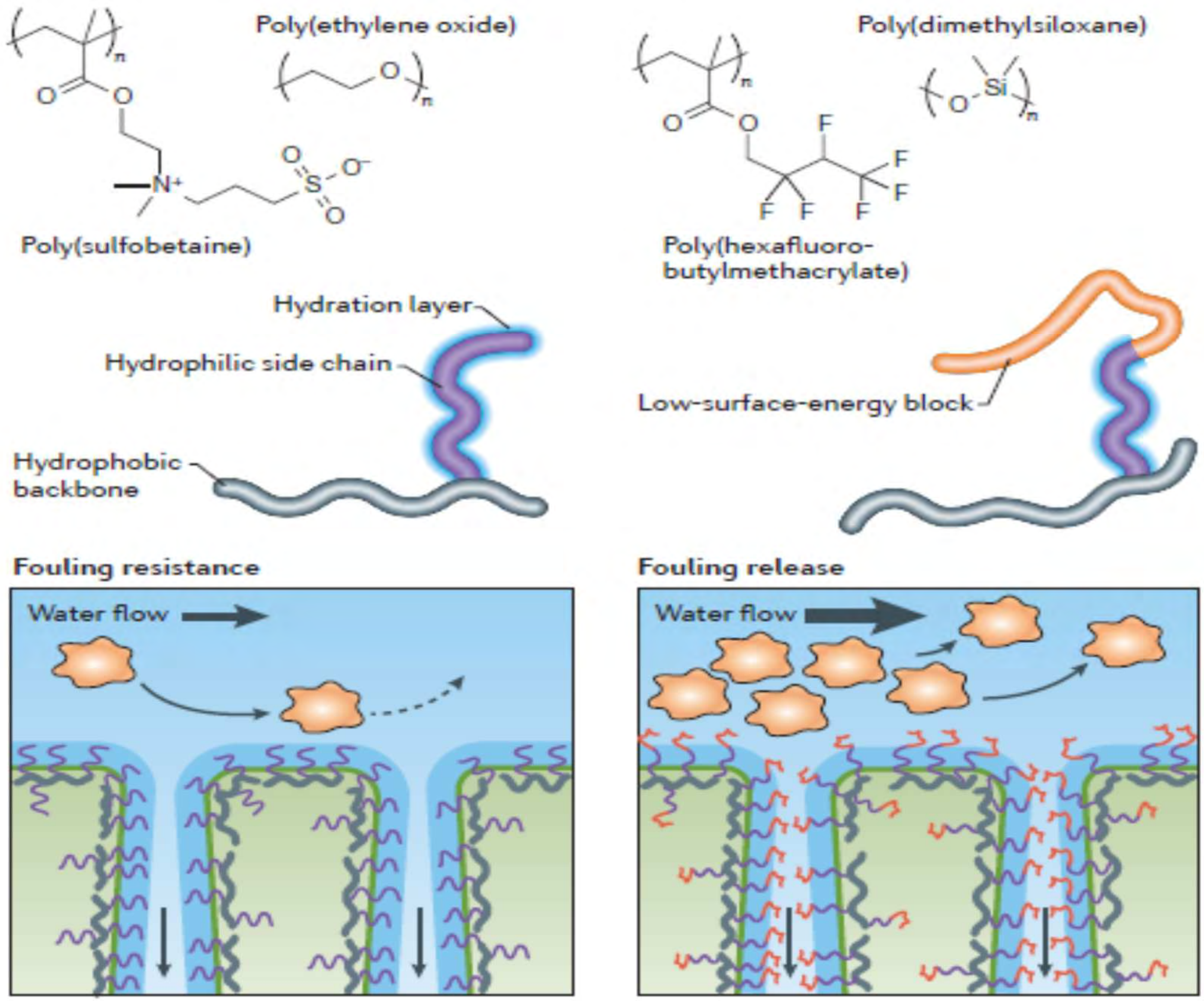
L, W, and H denote the length, width, and height of the channel, respectively; u(x, t) and v(x, t) are the cross and permeate flow velocities, respectively, with the local position (x), which is the distance from the inlet, and the operating time (t).
The channel length (L) can be increased according to the number of RO membrane elements (n) in a vessel for customary practice with several modules in series.

Polymer-based Nanostructured Membranes

- Polymeric materials and self-segregation approach for fouling minimization

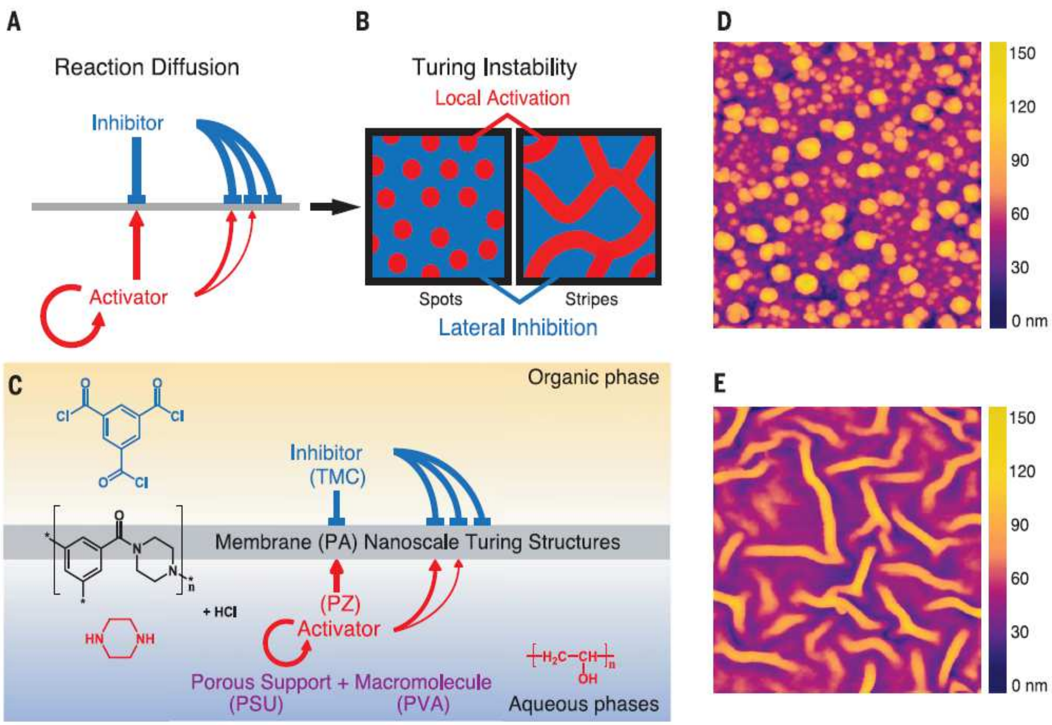
Hydrophilic polymers

Polymers with low surface area

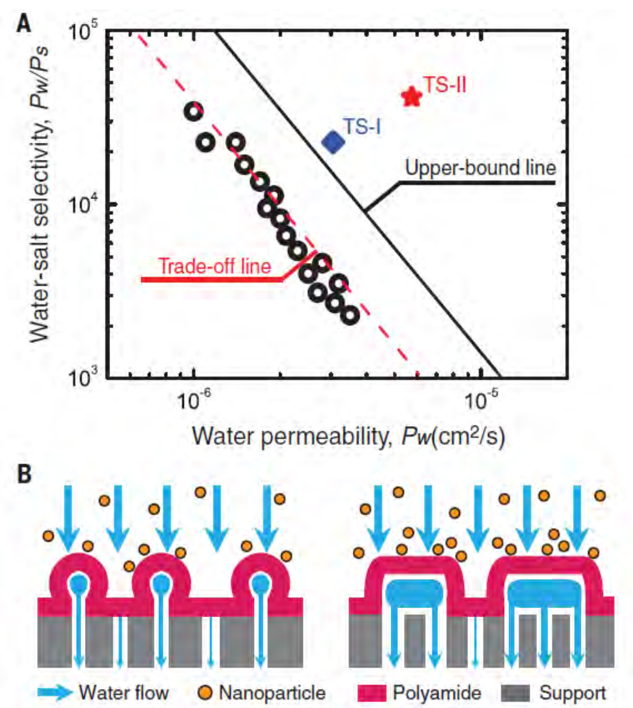


Polymer-based Nanostructured Membranes

- Turing-type membranes for water purification to increase water permeability
  - ✓ Turing-type polyamide membranes for water purification following a facile route based on interfacial polymerization.
  - ✓ Manipulation of shapes by control of reaction conditions enables the creation of membranes with bubble or tube structures.
  - ✓ Excellent water-salt separation performance that surpasses the upper-bound line of traditional desalination membranes and have high water permeability sites in the turing structures, where water transport through the membranes is enhanced.



Turing-type structures in interfacial polymerization



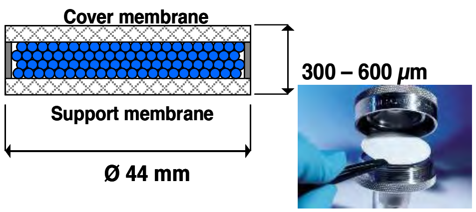
Spatial distribution of water permeability sites in the Turing-type PA membranes

Tan et al., Science, 2018

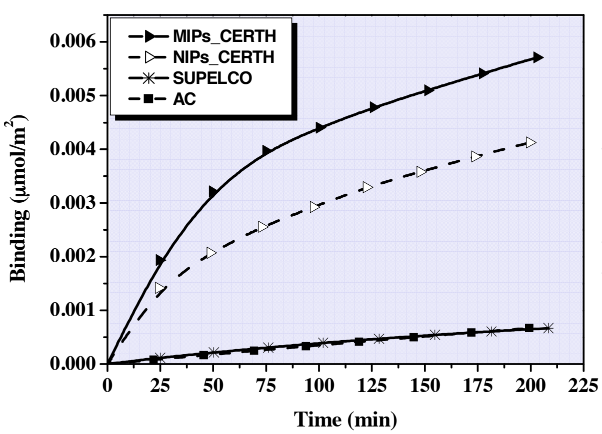
MIP-based Composite Membranes

- The incorporation of molecularly imprinted nanomaterials into membranes and filters offers several compelling opportunities, such as high selectivity.

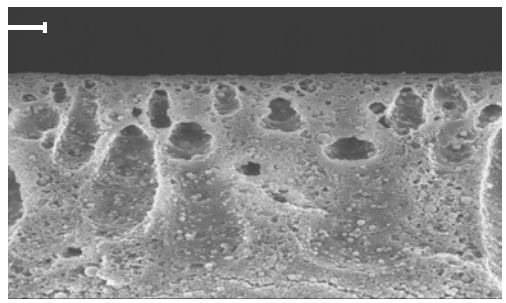
Sandwich Type Membranes with MIP NPs

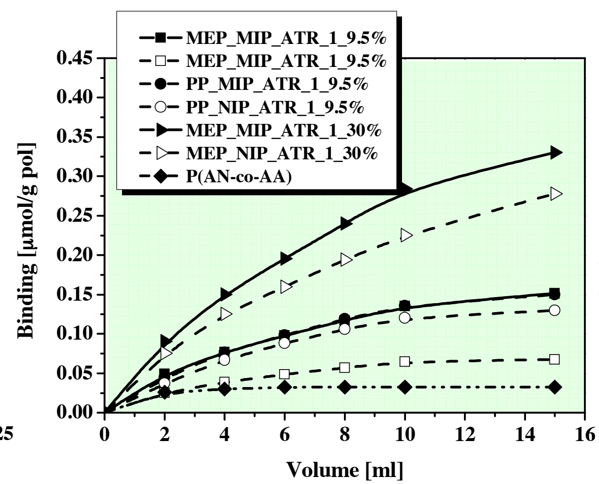


Comparison with packing materials:
C-18 SUPELCO and
activated carbon (AC) Ardrich

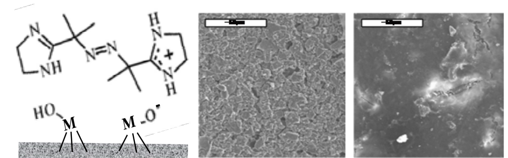


Phase Inversion Membranes with MIP NPs

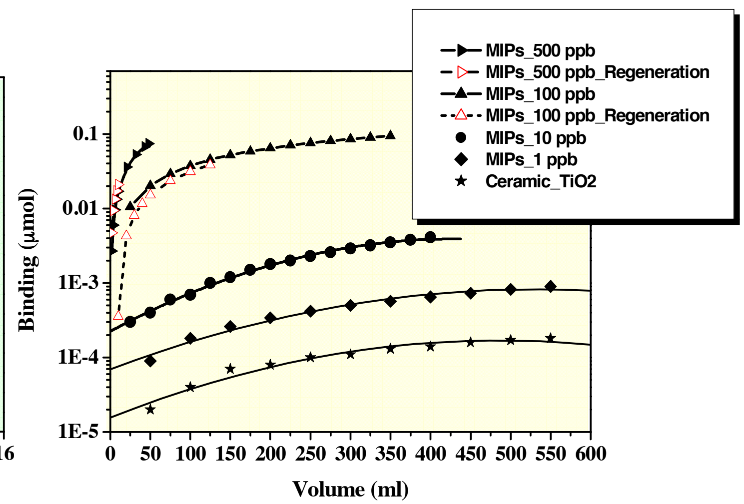




MIP Composite / Ceramic Membranes

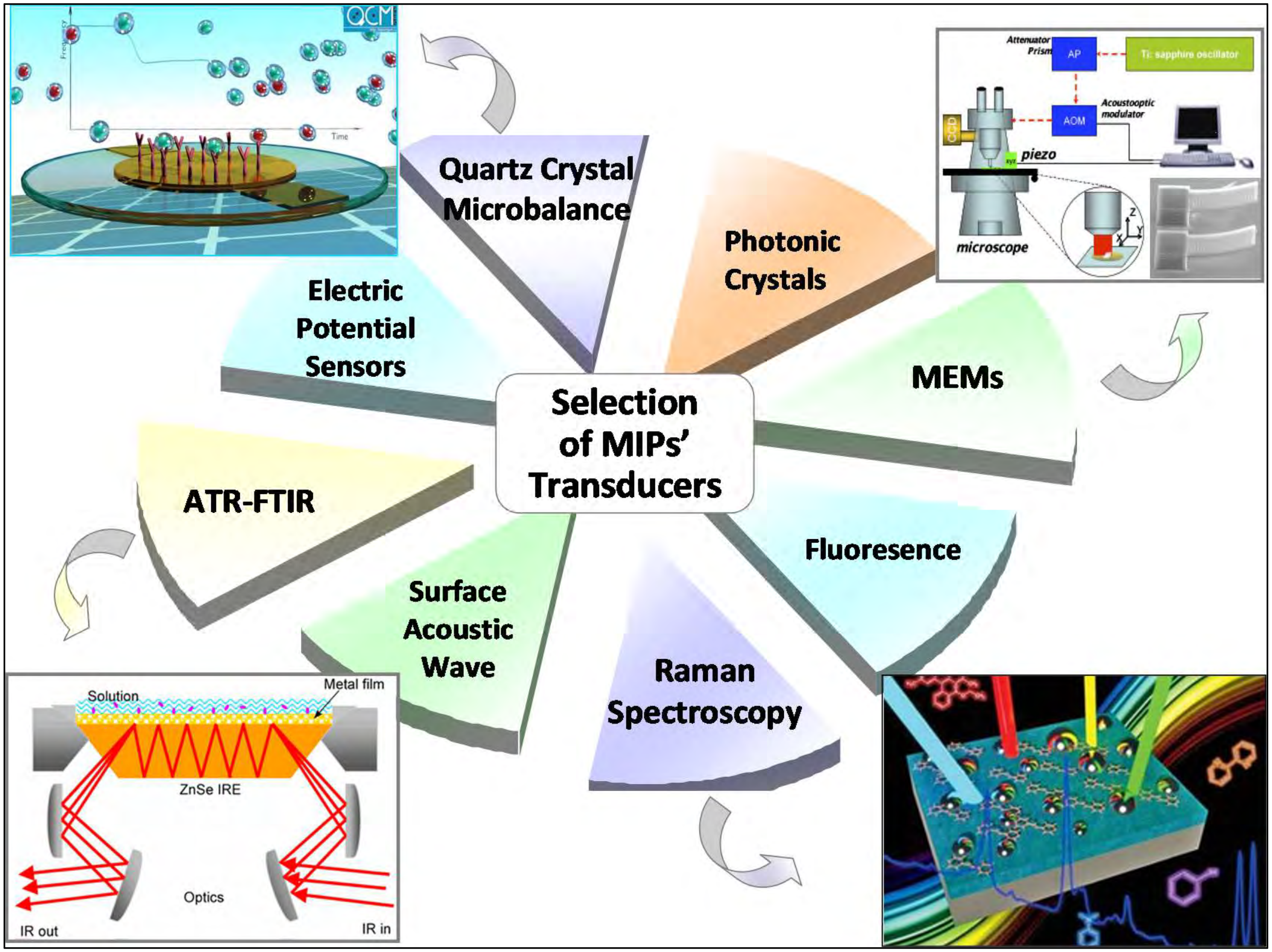


Before Grafting After Grafting



MIP-based Sensors

➤ Molecular imprinting for sensor applications and environmental monitoring.

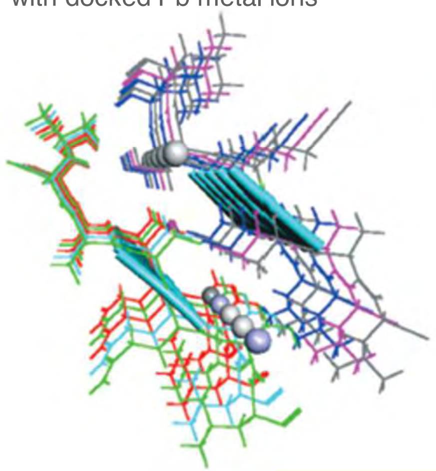


Bioinspired Composite Membranes

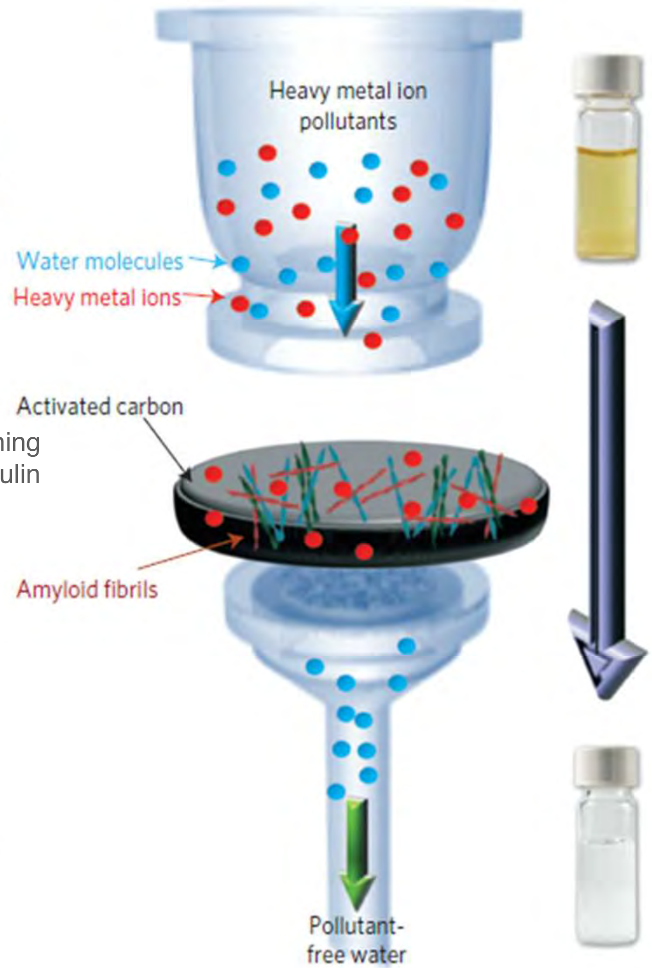
Amyloid–carbon hybrid membranes for universal water purification

Structure of the β-lactoglobulin protein with the strongest heavy metal-binding motif highlighted, 121-cys, with a lead ion attached

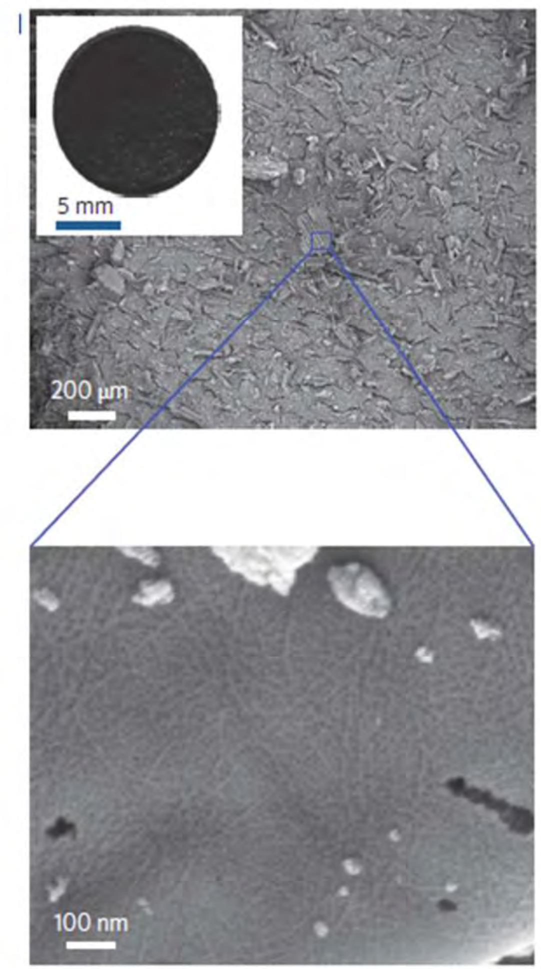
Amyloid-forming 121-cys-containing fragment (LACQCL) from β-lactoglobulin with docked Pb metal ions



Schematic representation of heavy metal ion purification by amyloid–carbon membranes, and photographs of Na_2PdCl_4 solution changing colour from yellow to colourless after filtration



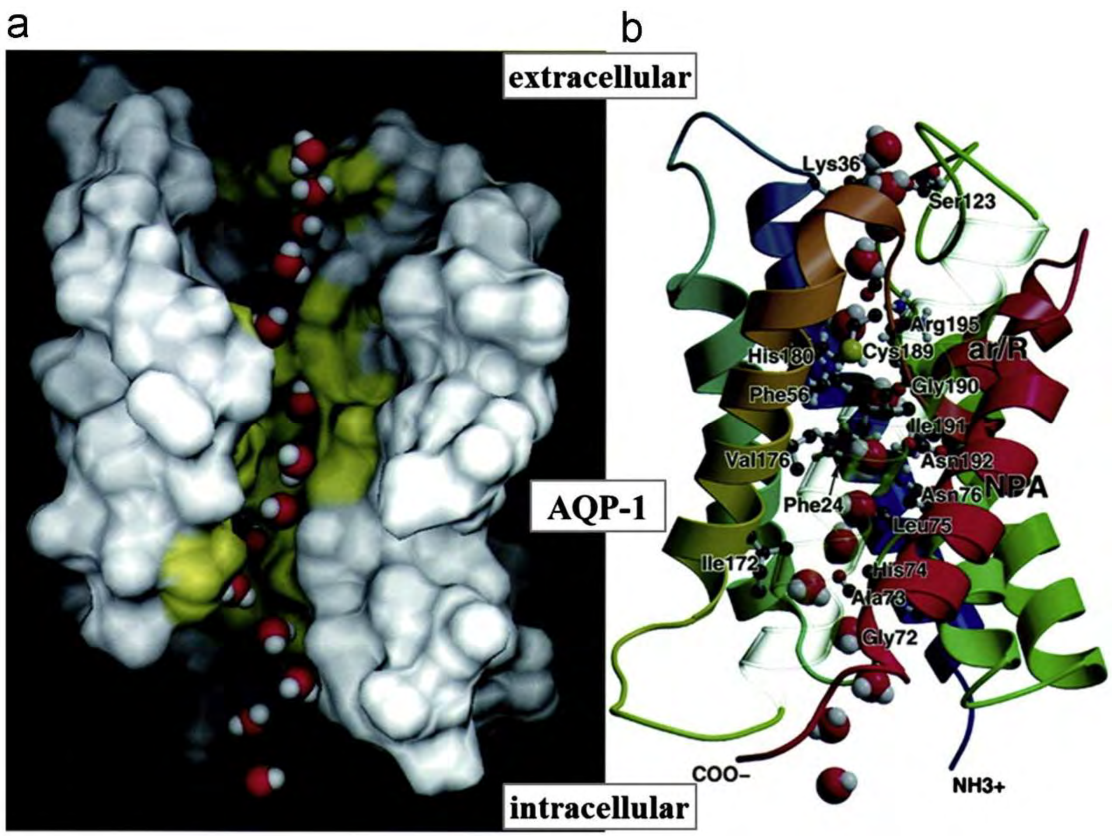
SEM image showing the surface of the composite membrane, with the visual aspect of the membrane shown in the inset



Bolisetty and Mezzenga, Nature Nanotechnology, 2016.

Molecular Dynamics for Optimization

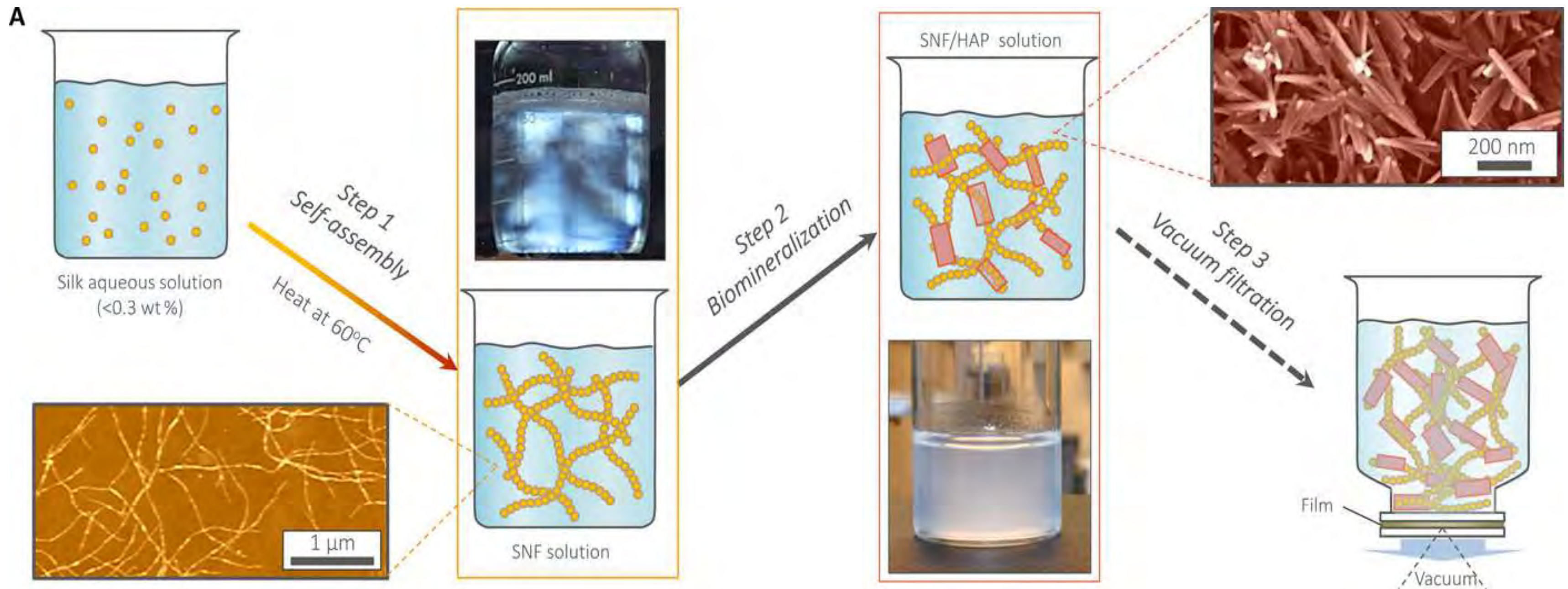
- Water passing through aquaporin-1, depicted in (a) surface representation and (b) ribbon representation, and simulated for 3.3 ns.
- Because of their excellent water conducting property, research on how to incorporate aquaporins into synthetic membranes has been carried out. It was found that the inclusion of aquaporin-Z into a polymeric membrane increased the water productivity of a pure polymer by approximately 800 times. In 2008, a US EPA research project attempting to develop a sustainable low energy membrane technology for desalination and contaminant removal involved aquaporin-Z.



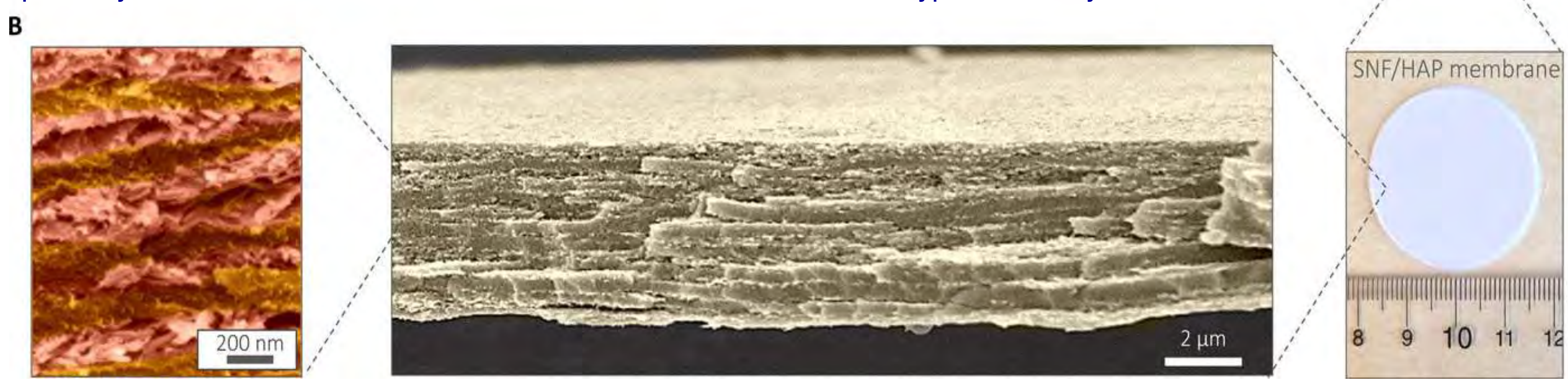
Ebro et al., 2013

Biomimetic Multilayer Membranes

Design and function of biomimetic multilayer water purification membranes



The pathway to fabricate the SNF/HAP* membranes and visualization of typical multilayer structures formed

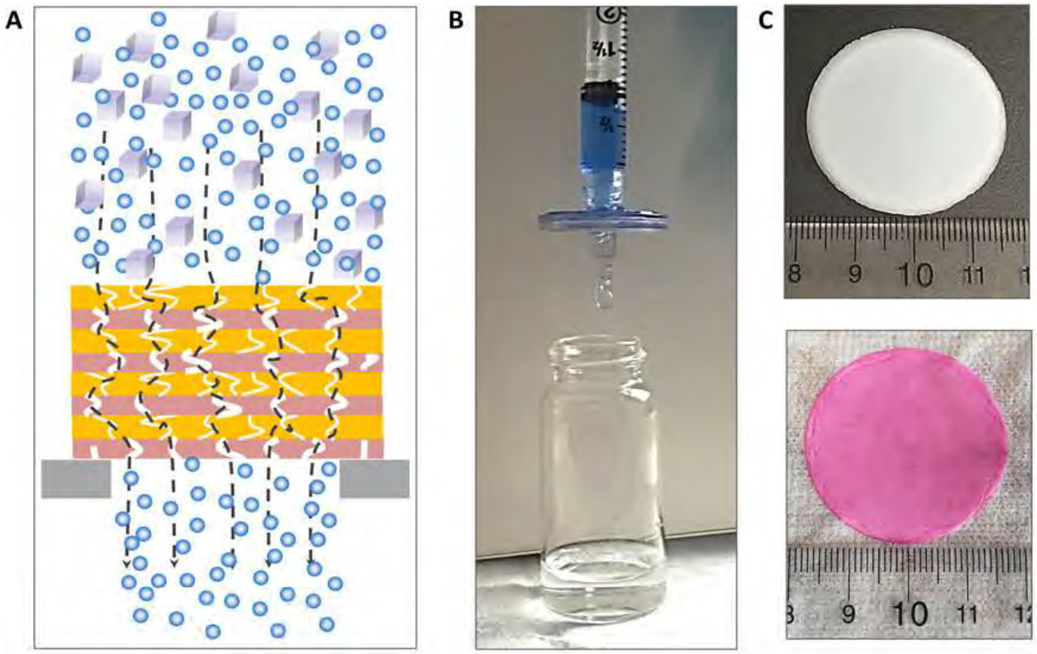


* silk nanofibril (SNF) and hydroxyapatite (HAP)

Ling et al., Science Advances, 2017.

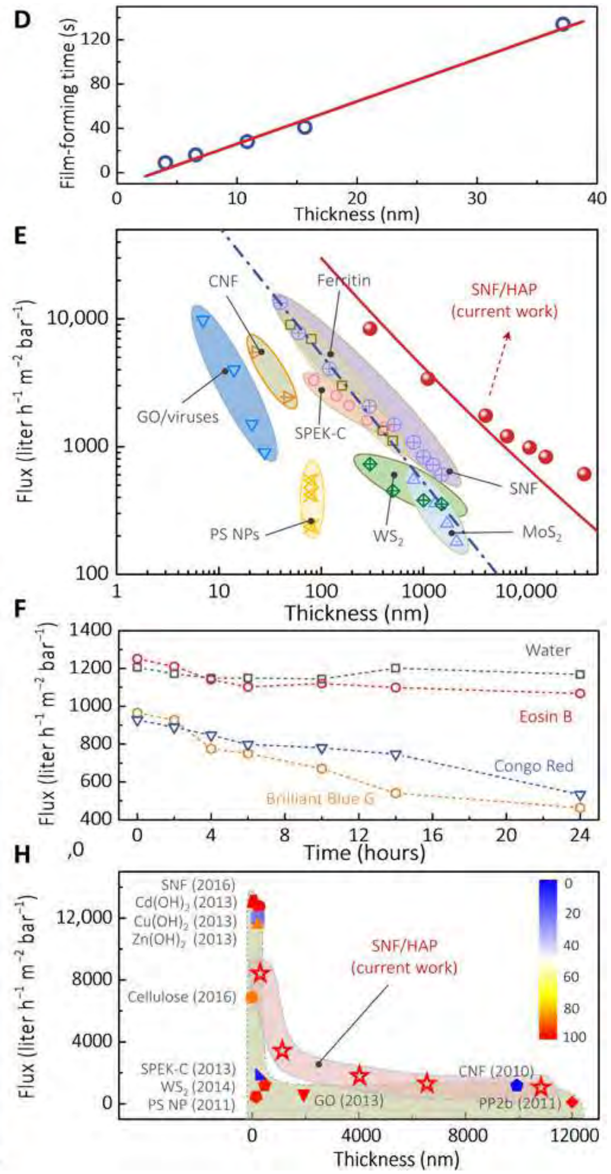
Biomimetic Multilayer Membranes

Separation performance of SNF/HAP membranes



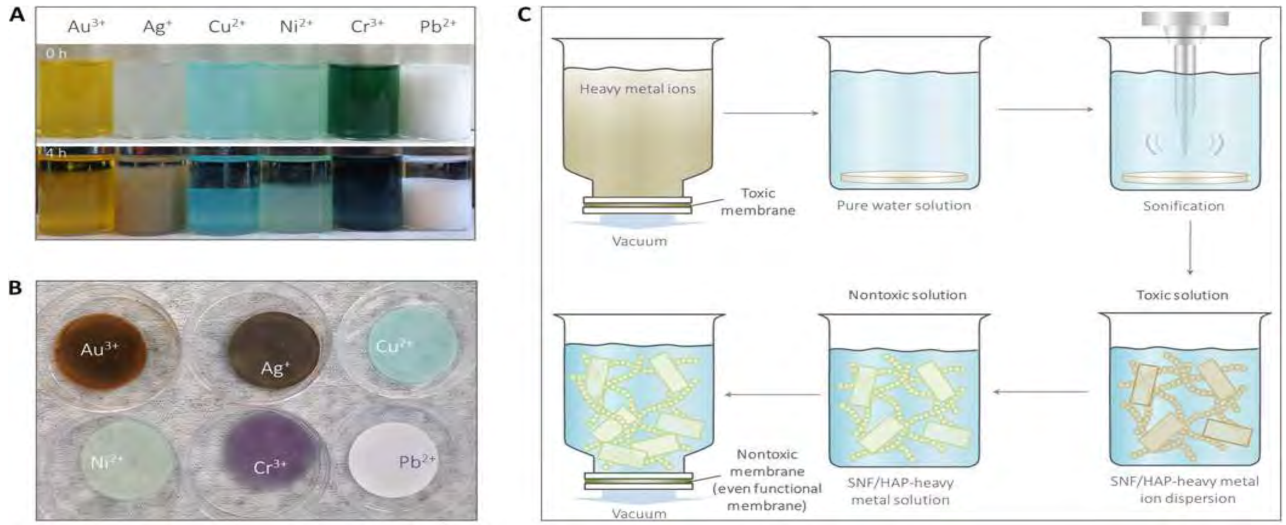
G Separation performance of 7-µm-thick SNF/HAP membranes for model compounds.

	Concentration	Flux (liter h^{-1} m^{-2} bar^{-1})	Rejection at 10 min (%)	Rejection at 2 hours (%)	Rejection at 24 hours (%)
Green fluorescent protein	0.05 mg ml^{-1}	1079.4	91.1	92.6	-
Cytochrome c	2.0 mg ml^{-1}	1253.6	97.8	61.8	-
Bovine serum albumin	2.0 mg ml^{-1}	635.9	70.2	33.3	10.7
Gold nanoparticles	~5.5×10^{13} unit per ml	1185.4	100	100.0	-
Eosin B	251 µM	1287.6	64.9	57.0	13.5
Orange G	306 µM	1015.4	76.7	32.1	18.7
Alcian Blue 8GX	80 µM	881.4	100	100	100
Brilliant Blue G	139 µM	927.9	100	100	100
Brilliant Blue R-250	44 µM	686.8	100	99.8	99.8
Alizarin Red S	434 µM	819.1	99.3	91.1	88.8
Rhodamine B	171 µM	1106.8	100	49.3	40.8
Congo Red	153 µM	964.8	100	100.0	90.9
Direct Red 81	240 µM	1019.7	99.8	88.3	56.4
Fluorescent Brightener 28	85 µM	1145.0	100	93.7	92.2



Biomimetic Multilayer Membranes

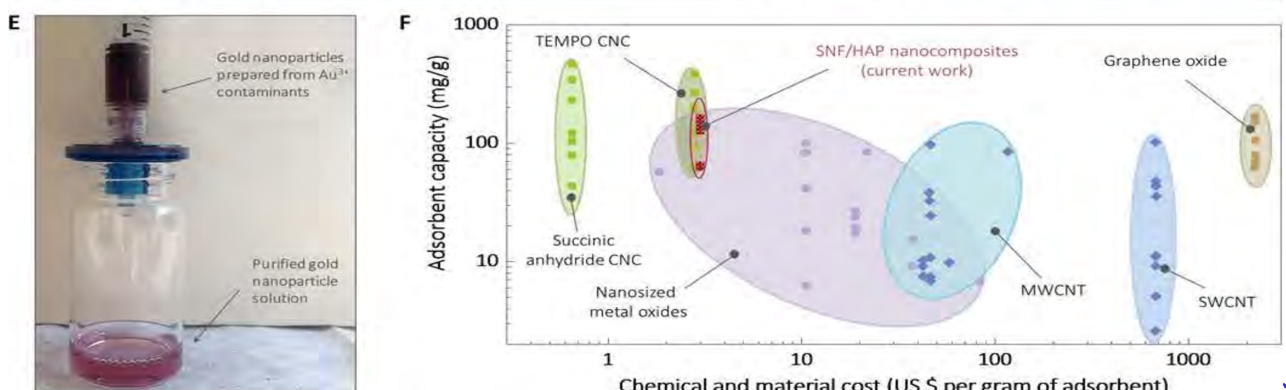
Removal and recycling of heavy metal ions by SNF/HAP membranes



D

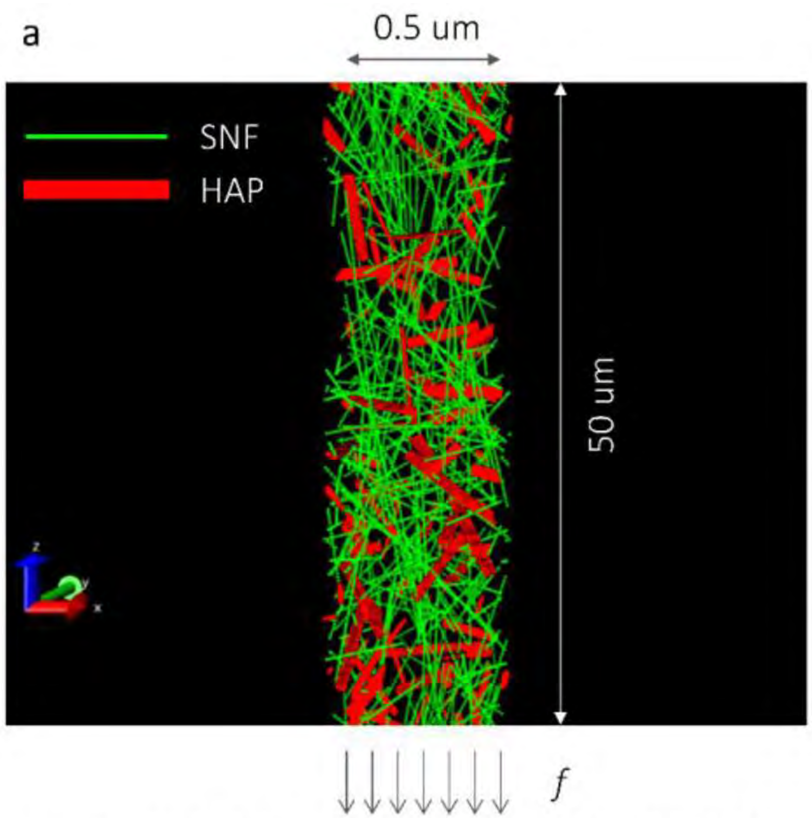
Separation and adsorption performance of SNF/HAP nanocomposites for heavy metal ions.

	IARC classification	Guideline for drinking water quality (mg/l)	Removing capacity of membrane (mg/g)	Maximum adsorption capacity (mg/g)	Postprocessing method	The materials prepared from postprocessing	Potential recycle application
Au^{3+}	–	–	135.7	164.2	Illumination Hydrothermal	Gold nanosheets Gold nanoparticles	Electronics Catalyst
Ag^{+}	–	–	–	–	Illumination	Ag nanoparticles	Antibacterium
Cu^{2+}	–	2	64.7	136.8	$NaBH_4$ reducing Adding NaOH	Cu nanoparticles CuO nanocrystals	Electronics Electrode
Ni^{2+}	Group 1	0.07	63.0	132.5	$NaBH_4$ reducing	Ni nanocrystals	Magnetic
Cr^{3+}	Group 3	0.05	126.7	145.8	Adding NaOH	Cr_2O_3	Pigment
Pb^{2+}	Group 2A	0.07	–	–	Reaction with H_2S gas	PbS nanoparticles	Catalyst



Molecular Dynamics for Optimization

- Simulation setups and related parameters for SNF/HAP assembly and deposition modeling. The simulation setups (a) and related parameters (b) for SNF/HAP assembly and deposition modeling.



Subjected to a gravity field that accounts for the drag force from the water flow

b

$f_{drag} = -6\pi\mu R v$

The bead radius is given by $R_{silk} = (\frac{3}{4} * (d^2 r_0/4))^{1/3} = 5.72$ nm, $R_{Hap} = (\frac{3}{4\pi} * t^3)^{1/3} = 3.72$ nm, for $v = 250$ m/s

$f_{drag\_silk} = -6\pi\mu R v = 333.8$ kcal/mol/A

$f_{drag\_hap} = -6\pi\mu R v = 217.1$ kcal/mol/A

$a_{drag\_silk} = 0.00055$ kcal/mol/A/amu

$a_{drag\_hap} = 0.00085$ kcal/mol/A/amu

* silk nanofibril (SNF) and hydroxyapatite (HAP)

Ling et al., Science Advances, 2017.

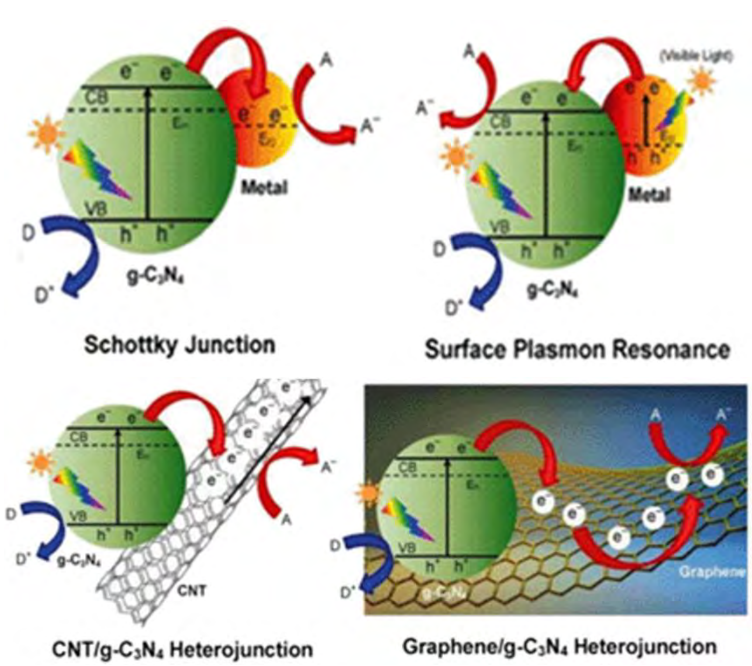
Nano-photocatalysts

Nanophotocatalysts

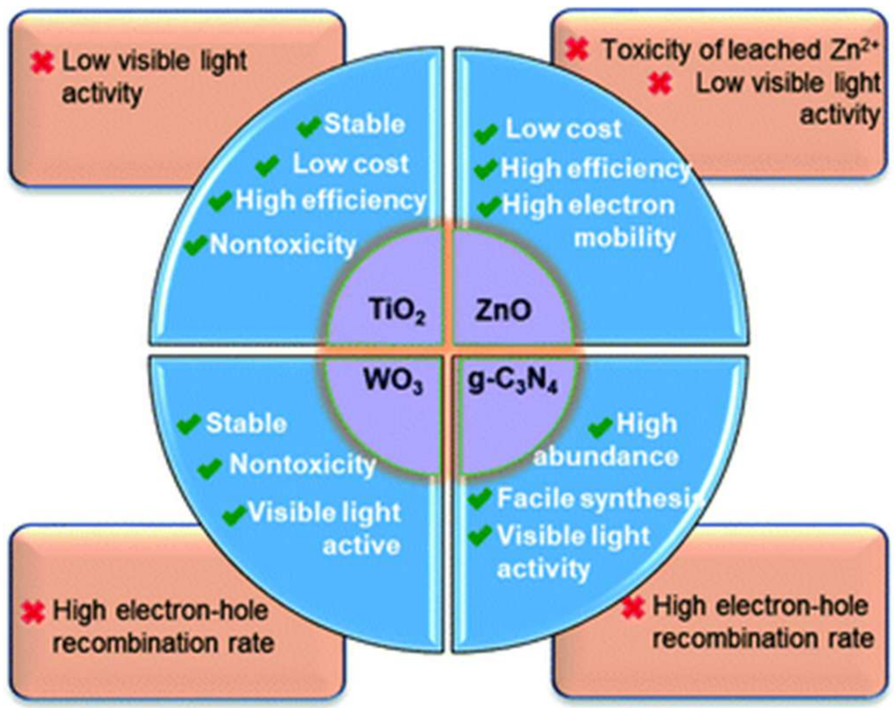
Advanced Oxidation Processes with Nanostructured Photocatalysts

- Advanced oxidation processes (AOPs) are defined as water and wastewater-treatment processes which involve the generation of hydroxyl radicals to effect water purification.
- In water-treatment application, AOPs have been mainly targeted to remove and degrade taste and odor-causing compounds, natural organic matters, pesticides, hormones, and pharmaceuticals which are introduced into water supplies from agricultural and industrial activities in trace amount.

Photocatalysis - Modification Methods



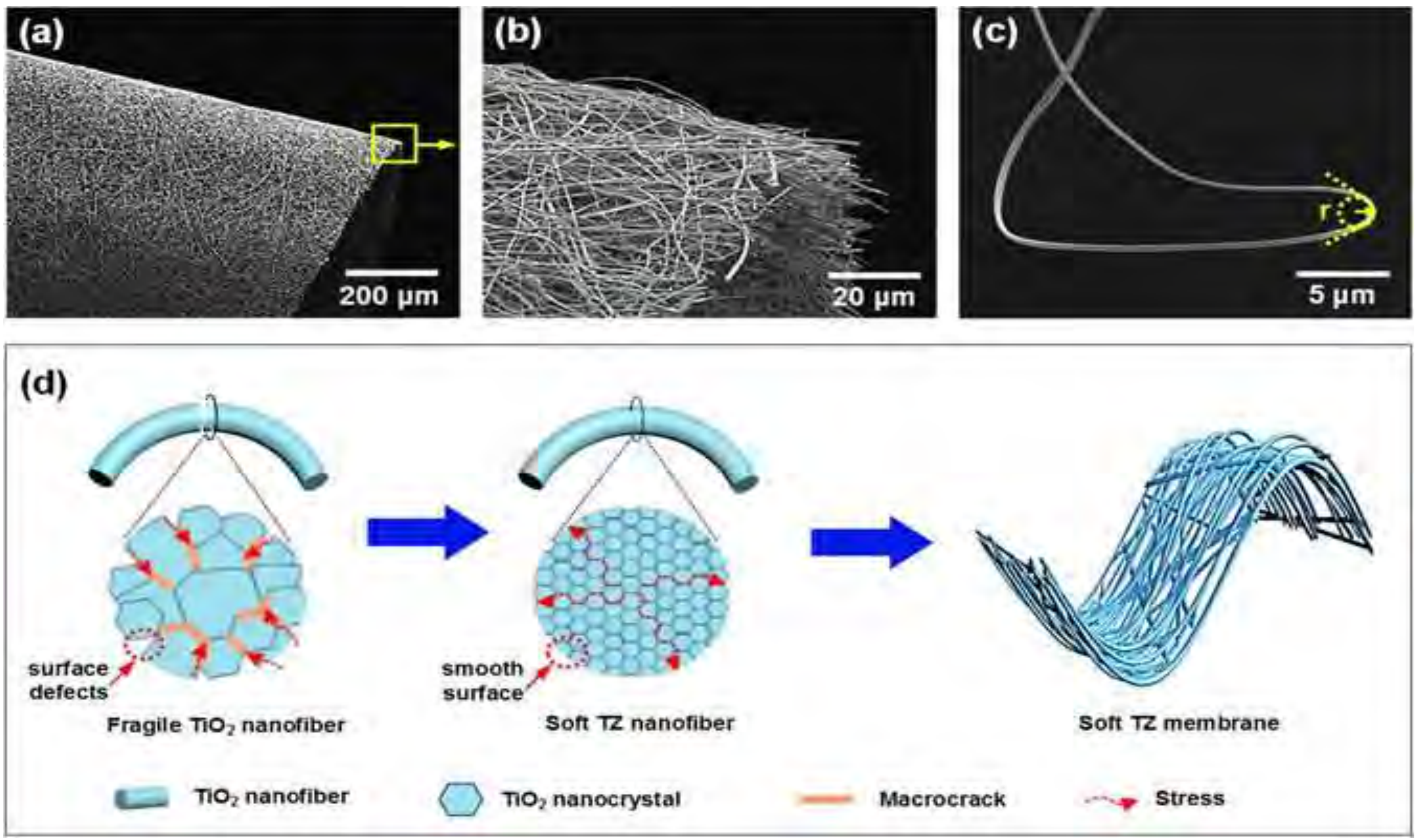
Merits and shortcomings



Titanium-based Nanofibrous Membranes

- Soft Zr-doped TiO_2 Nanofibrous Membranes with Enhanced Photocatalytic Activity for Water Purification

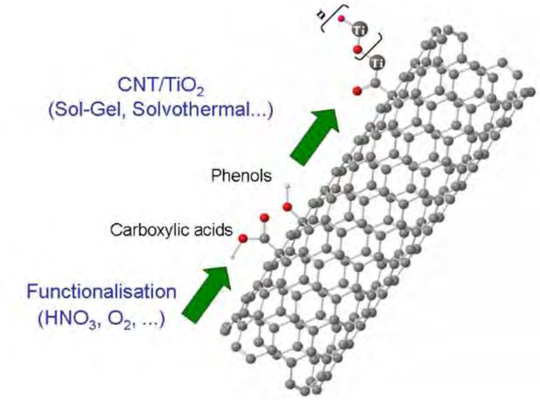
Song et al., Scientific Reports, 2017.

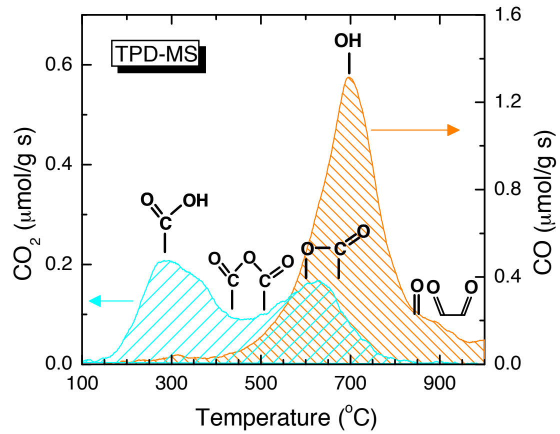


(a) SEM image of the bended TZ-10 nanofibrous membranes. (b) The high magnification SEM image of selected area in (a). (c) SEM image of bended single TZ-10 nanofiber. (d) Schematic illustration showing the probable mechanism of the softness of TZ membranes.

Composite CNTs/Titania Nanostructures

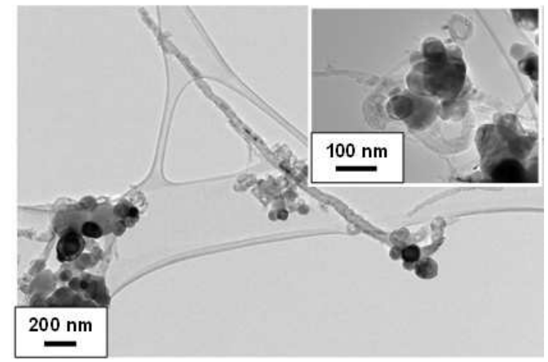
- Controlled generation of oxygen functionalities on the surface of SWCN by HNO_3 hydrothermal oxidation



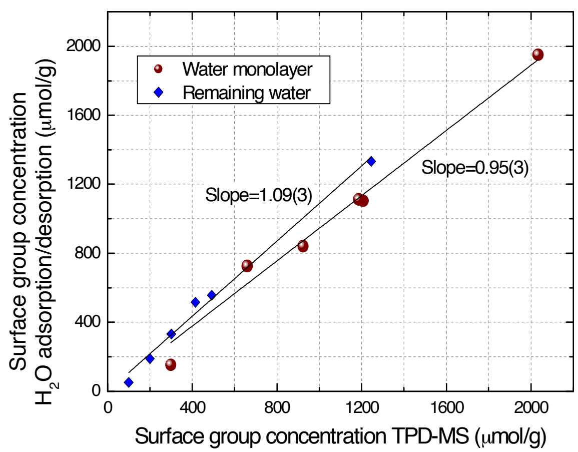


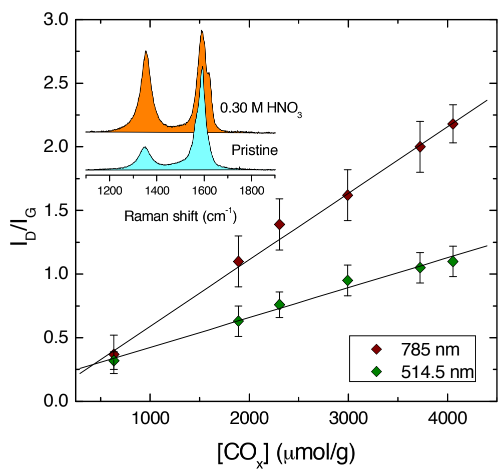
Carbon 48 (2010) 1515-1523

- Carbon nanotube $–TiO_2$ composites



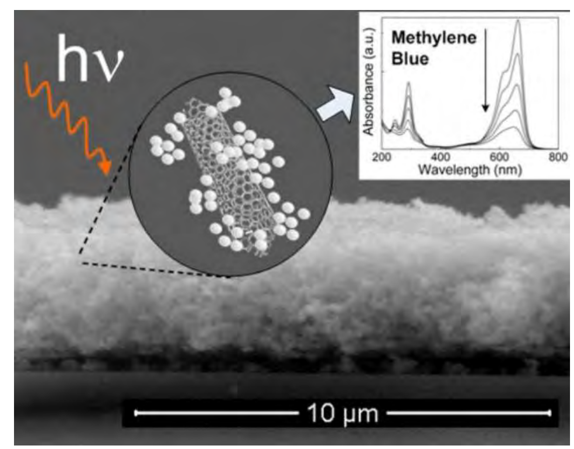
- Controlling and quantifying oxygen functionalities on hydrothermally and thermally treated SWCNT.





J. Phys. Chem. C 115 (2011) 8534–8546

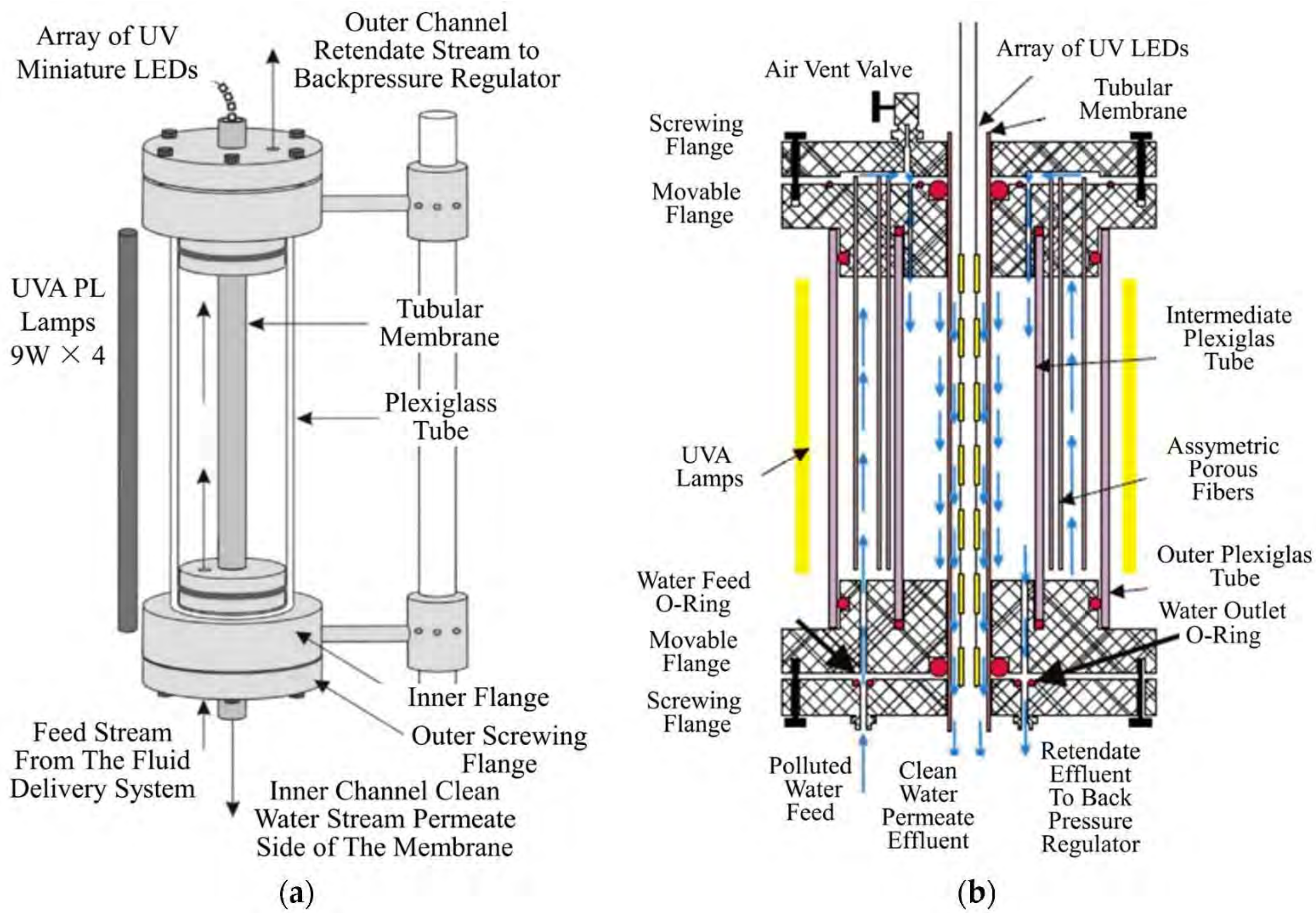
- Carbon nanotube$–TiO_2$ thin films for photocatalytic applications



Catalysis Today 161 (2011) 91-96

Applications & Process Optimization

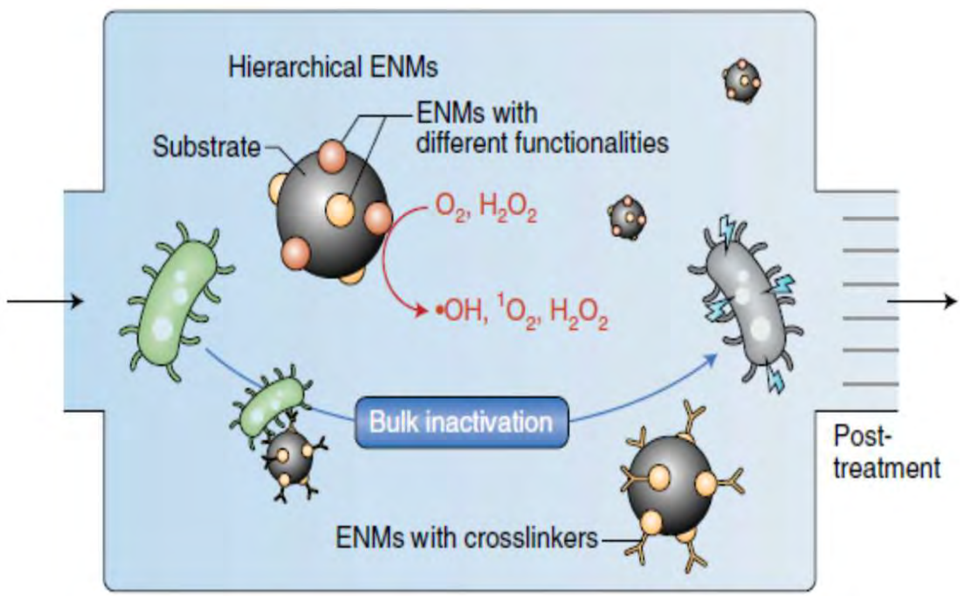
- Schematic diagram of a (**a**) primary; (**b**) improved continuous flow PMR with double-side active TiO_2 modified membrane for water purification.



Zheng et al., 2017

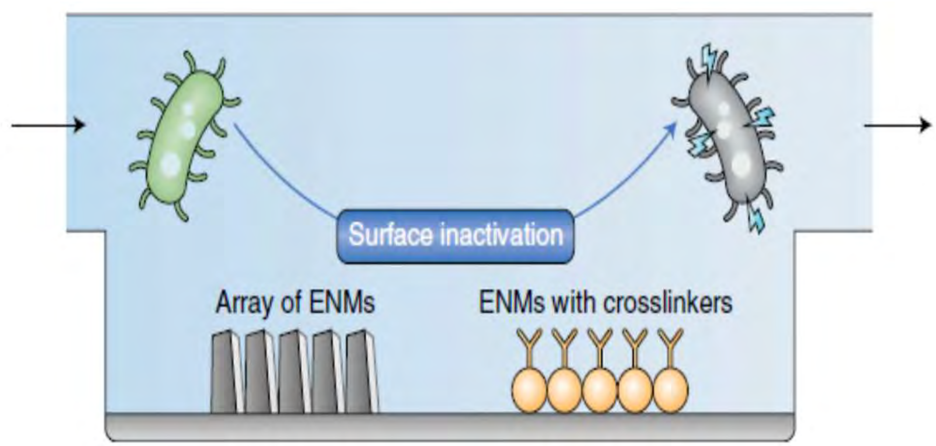
Water Disinfection

ENM-Enabled Disinfection Processes

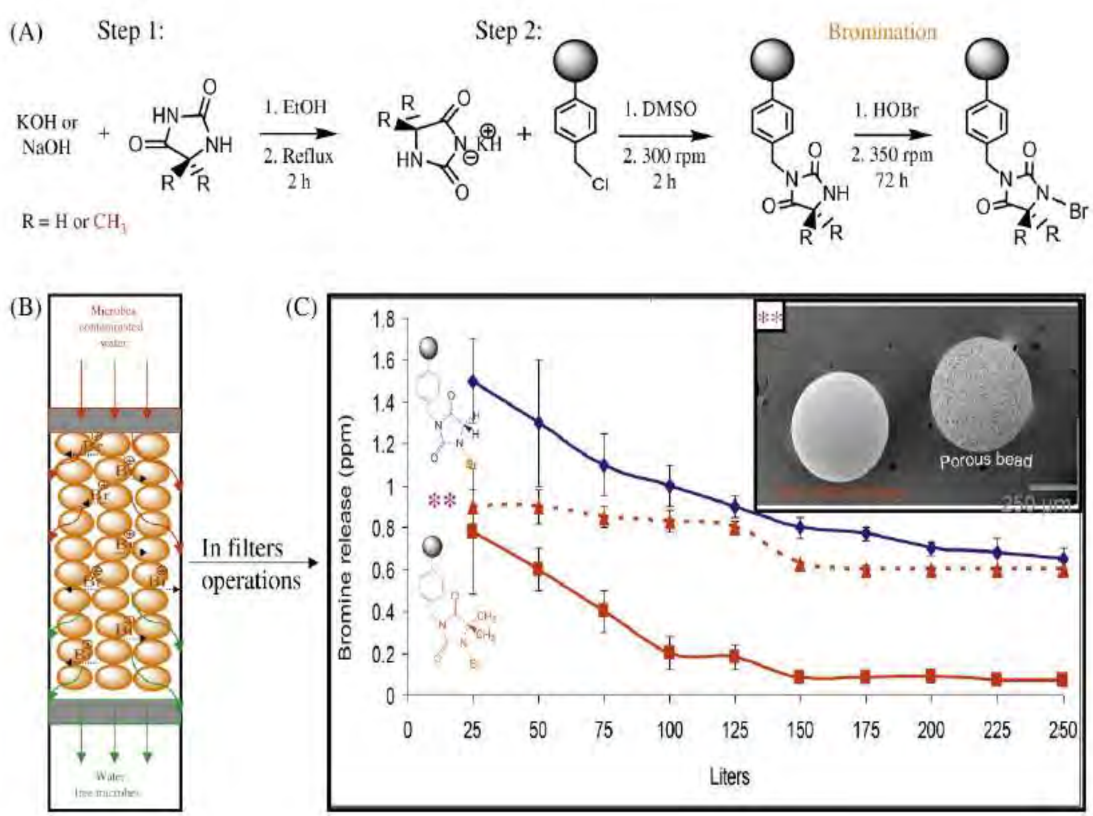


- ✓ Suspension of multifunctional ENMs in a reactor and subsequent ultrafiltration to prevent ENM release to the product water, typically operated in a recirculation mode.
- ✓ ENMs produce reactive oxygen species photocatalytically or electrocatalytically that oxidatively inactivate pathogens or specifically interact with pathogens via crosslinkers to damage cell-wall structure and function.

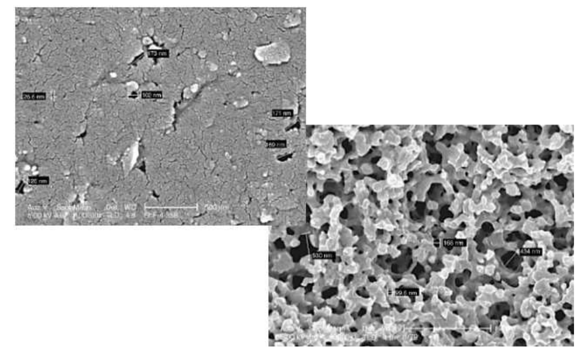
- ✓ Surface-immobilized ENMs. The ENMs exert similar inactivation mechanisms as the suspended ENMs or their unique alignment leads to passive inactivation via cell-wall interaction.
- ✓ Pathogen transport from the bulk phase toward ENM surface is the key design consideration.



Nano-Antimicrobial Polymers



(A) N-bromo-hydantoin synthesis by conjugation to microbeads followed by bromination; (B) filters loaded with N – bromo – hydantoin / 5,5' – dimethylhydantoin - PS beads; and (C) hypobromous release from different beads having different characteristics



- ✓ This resin exhibited excellent antimicrobial properties; 6- and 4-log reduction for E. coli and MS2, respectively, were obtained for all tested points during 250 L.
- ✓ This brominated resin should be considered in filters for decontamination of drinking water. These materials were found to have great potential due to ability to decontaminate large volumes of contaminated water, low costs, and bromine rechargeability.

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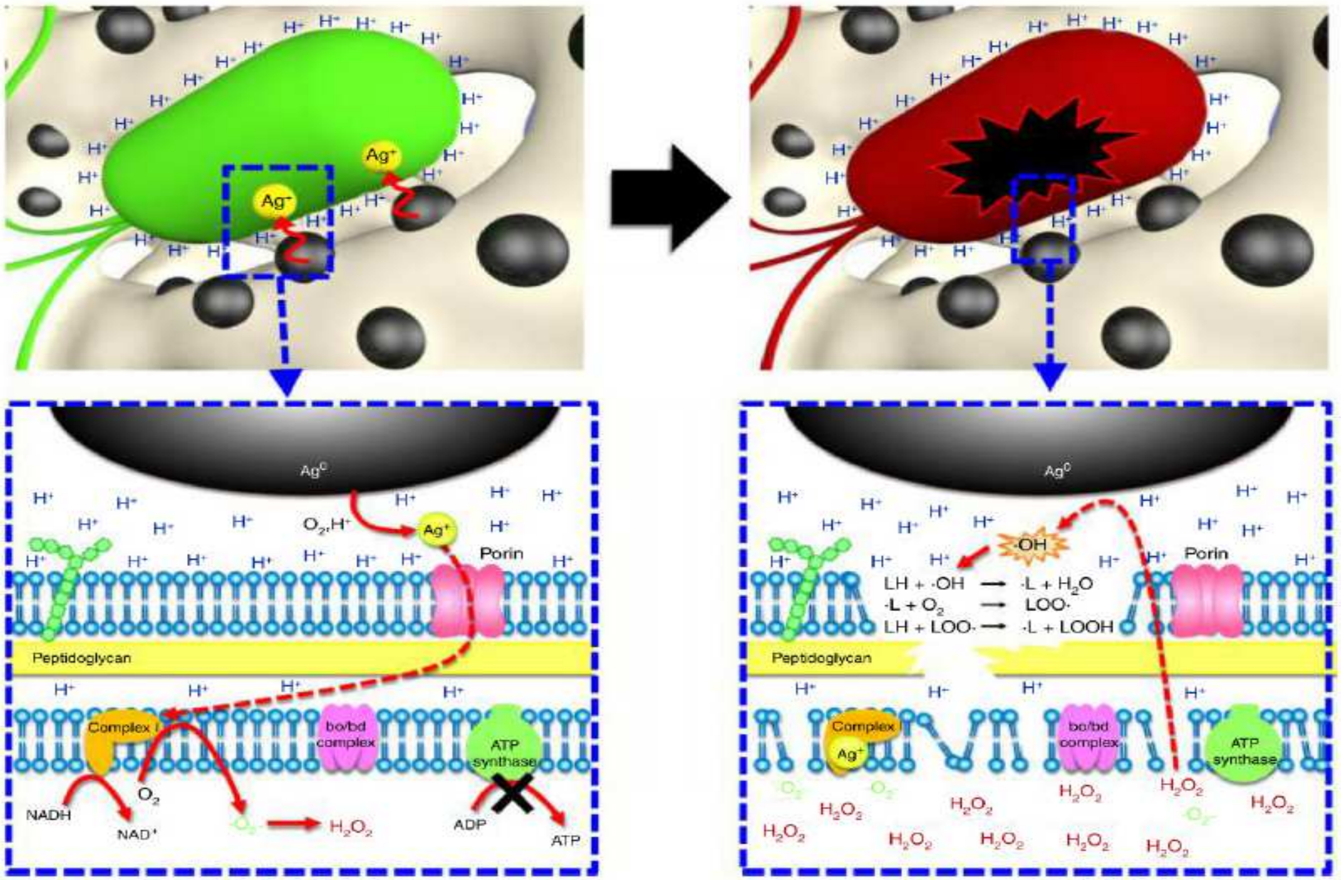
Silver Nanoparticles

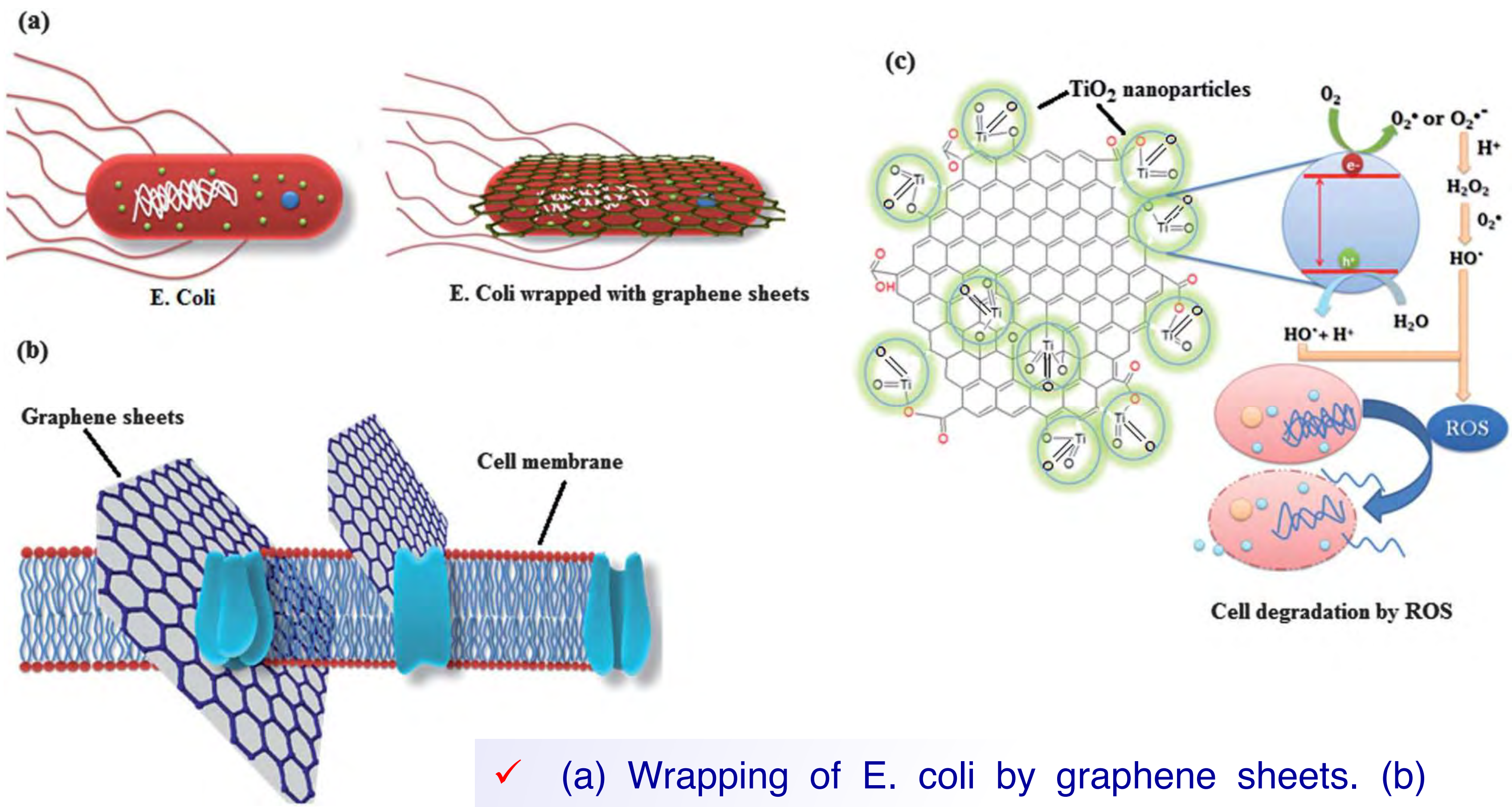
Bactericidal mechanism of Ag NPs

Water Purification, 2017



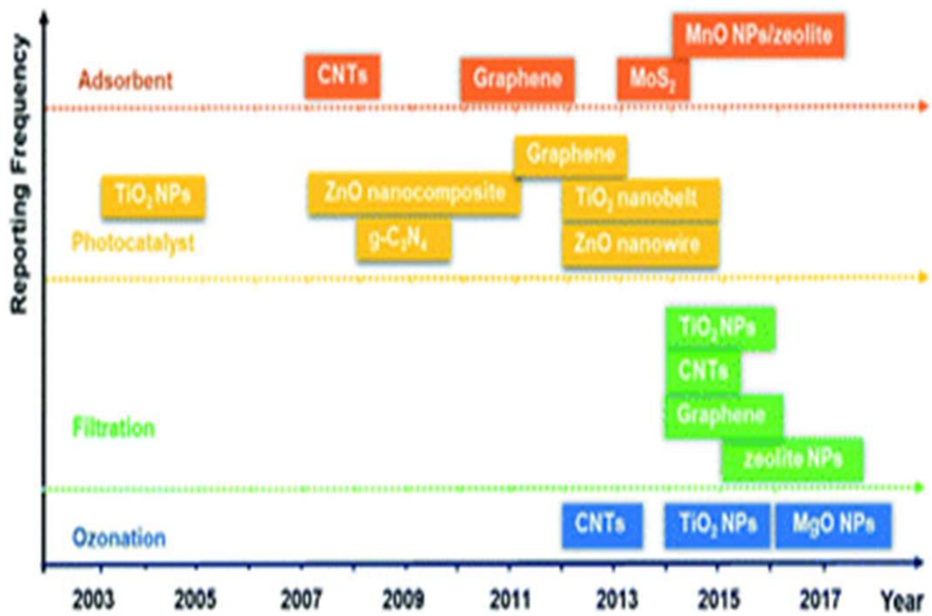
✓ Ag+ is taken up by the bacteria and disturbs ATP synthesis and the electron transport chain. The latter mechanism is the indirect formation of ROS. The hydroxyl radicals, generated via decomposition of H2O2, can initiate a peroxidative sequence that inevitably results in cell death by destroying the cell membrane (·L and LOO· are a carbon-centered radical and a peroxyl radical, respectively.

Carbon-based Nanomaterials



- ✓ (a) Wrapping of E. coli by graphene sheets. (b) Slicing of cell membrane by sharp edges of graphene. (c) Mechanism involved in photoinactivation of cells by metal oxide/graphene composite.

Metrics



➢ Water purification has been one of the most dynamic research fields in recent years with significant impact on the medical and environmental research with near 5000 papers as indexed by the Science Citation Index-Expanded (SCIE) as of December 2015.