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Leiden
The Netherlands

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Andrieu-Brunsen, A.; Azzaroni, O.; Binyaminov, H.; Danil de Namor, A.; Fyta, M.; García-Martínez, J.; ... ; Toimil-Molares, E.

Citation

Andrieu-Brunsen, A., Azzaroni, O., Binyaminov, H., Danil de Namor, A., Fyta, M., García-Martínez, J., ... Toimil-Molares, E. (2026). The Power of Tiny Spaces. *Jacs Au*, 6(8), 4353-4366. doi:10.1021/jacsau.6c00663

Version: Publisher's Version

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Downloaded from: <https://hdl.handle.net/1887/4310364>

Note: To cite this publication please use the final published version (if applicable).

The Power of Tiny Spaces

A. Andrieu-Brunsen,* O. Azzaroni,* H. Binyaminov, A. Danil de Namor, M. Fyta, J. García-Martínez, S. Guldin, S. Howorka, S. Lamotte, S. G. Lemay, B. V. Lotsch, S. Magdassi, K. Nakanishi, C. Plueg, S. Polarz, L. Pozzo, M. Rafti, M. Rehahn, A. G. Roth, C. Sanchez, D. A. Scherlis, G. J. A. A. Soler-Illia,* I. Szleifer, K. Tschulik, M. Thommes, and E. Toimil-Molares



Cite This: *JACS Au* 2026, 6, 4353–4366



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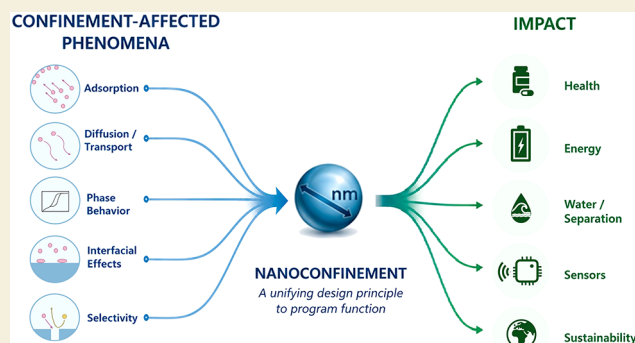
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ABSTRACT: Confined spaces at the nanoscale — pores, channels, and cavities that alter molecular affinities and restrict molecular motion, orientation and local distribution — are emerging as a powerful design principle for next-generation materials. By tailoring the structure and functionality of these confined spaces, it is possible to control reactivity, transport, and material properties in ways that are unattainable in bulk systems. This Perspective highlights nanoconfinement as a unifying principle for programming function and addressing major societal challenges in energy, water, health and sustainability. Drawing inspiration from nature's remarkable precision in bio-molecular control, we showcase six representative areas in which confined spaces are transforming technology: chromatography, catalysis, nanofluidics, bioinspired pore design, confinement-programmed material states, and data-driven material development. Together, these examples illustrate the power of nanoconfinement as an enabling unifying concept. By integrating orthogonal functionalization strategies, advanced characterization, modeling, and digitalization, programmable nanoconfinement will become a versatile framework for engineering materials and processes that meet the demands of a sustainable and technologically advanced society.

KEYWORDS: confinement, nanopore, energy, medicine, separation, catalysis, sustainability, data-driven material design, nanofluidics, bioinspired materials



INTRODUCTION: HOW NANOCONFINEMENT TRANSFORMS MATERIAL FUNCTION

Global society faces major challenges: clean water is becoming increasingly scarce, energy must be generated more sustainably,^{1–4} and healthcare demands more precise diagnostics and more targeted therapies. At the same time, essential raw materials are finite, and decarbonization requires new technological solutions (Figure 1). Addressing these challenges in energy, water, health, sustainability, and circularity requires a fundamental rethinking of how to design materials and technological processes.

We propose nanoconfinement as a unifying design principle for next-generation materials. Rethinking material design from the “tiny” spaces within materials or metamaterials covers nanocavities, channels, and nanopores with diameters ≤ 100 nm.⁵ Rather than considering material geometry, topology and interfacial chemistry as separate parameters, we argue that these should be integrated under the concept of nanoconfinement to control how molecules behave within the restricted spaces. This includes whether and how molecules move, fold, assemble, react, maintain their hydration shell, or bind to

surfaces. Consequently, nanoconfinement influences the state, phase, diffusivity, conductivity, and wetting behavior as emergent tunable functional properties that redefine intrinsic material constants at the nanoscale. As a result, nanoconfinement alters existing or even creates new phase transitions⁶ improves separation efficiency and reaction selectivity. The preferential stabilization of reactants leads to improved yields and minimized byproduct formation.^{7,8} Thus, nanoscale confinement acts via thermodynamics and kinetics to reshape energy landscapes, alter phase behavior, diffusion, and conductivity, and tunes reaction pathways.

Nature uses spatial confinement to perfection. Enzymes rely on tiny reaction pockets to steer chemical transformations while cell membrane pores precisely control molecular

Received: April 28, 2026

Revised: June 25, 2026

Accepted: June 29, 2026

Published: July 19, 2026





Figure 1. Impact of confinement on societal challenges in the areas of health, energy, water, and sustainability. The authors designed all scientific content, graphical elements, and overall structure of the figure. Artificial intelligence-assisted tools were used solely for color optimization.

transport, enabling water homeostasis in the eye, filtration in the kidneys, or selective translocation of molecules and ions

across membranes. Their remarkable efficiency arises from the finely tuned design of confined spaces at the nanoscale.⁹

The same fundamental principle is increasingly exploited in technology where nanoconfinement underpins applications ranging from chromatography and molecular filtration^{2,10} to catalysis,^{1,7} gas- and energy storage,⁴ and nanopore-based DNA sequencing.¹¹ More recently, these nanoconfinement concepts have been extended to protein analysis and the detection of disease-associated post-translational modifications,¹² and the characterization of glycans,¹³ and synthetic polymers. The importance of nanoconfined materials is also the 2025 Nobel Prize in Chemistry for nanoporous metal-organic frameworks (MOFs).

Although confined materials and metamaterials have already made significant contributions to energy, water, health, and sustainability, a systematic understanding of nanoconfinement remains lacking, particularly when confined space is viewed as an active design element that encodes functionality. Current research has highlighted the strong effect of confinement on material properties, yet confinement effects have so far been exploited as unintended byproducts rather than as a result of deliberate spatial design. This paradigm must shift now.

A transition toward confinement-programmed nanomaterials design presents considerable opportunities. By learning how to systematically design, shape and precisely arrange nanopore structures, it will become possible to control material properties with unprecedented accuracy, enabling improved sensors, more efficient catalysts, novel purification systems, and even chemical data storage. Achieving this vision requires a detailed understanding of how spatial structure, molecular

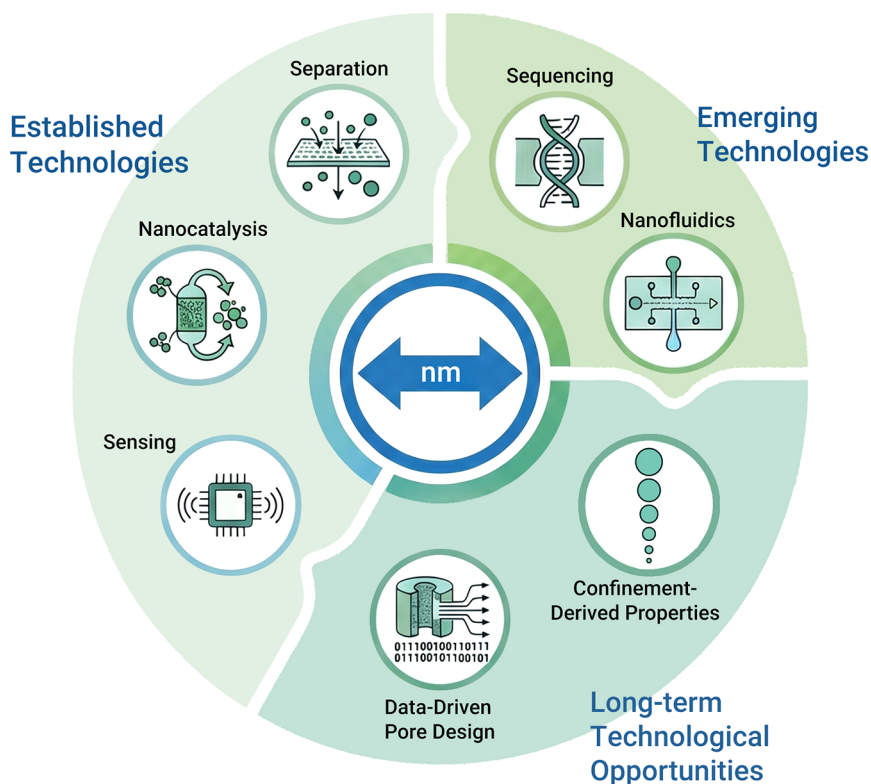


Figure 2. Existing and emerging technologies as well as long-term conceptual opportunities by rethinking design from the perspective of confined space. The depicted technologies refer to the six chosen paradigms discussed in the text. The authors designed the scientific content and overall structure of the figure. Artificial intelligence-assisted graphic design tools were used to refine the visual appearance, including color optimization and icon redesign.

behavior and material performance are interconnected on the nanoscale, and how these relationships can be harnessed in practical applications. Emerging approaches like big-data analysis, AI-based models, novel synthetic concepts, and the integration of nanopores into complex material systems promise solutions that surpass established technologies and may even enable new technological concepts. Ultimately, a deeper understanding of confinement will lead to technological innovations with the potential to tackle urgent societal challenges.

In the following sections, we discuss six representative areas where nanoconfinement is reshaping materials design and function, leading to improvements of existing and the development of new technologies which have not yet reached commercial implementation: chromatography, catalysis, nanofluidics, bioinspired pore design, confinement-derived material properties, and data-driven materials development (Figure 2). Together, these key topics illustrate how mastering nanoscale confinement can unlock technological pathways to address the societal challenges of green energy production, clean water generation, advanced healthcare and environmental sustainability.

Chromatography – Precise Pore Structures for Reproducible Performance

Challenge. Liquid chromatography is the standard method for analyzing and purifying molecules in industry and research from pharmaceuticals to environmental analysis. Each year, more than 800,000 separation columns are produced to serve over 220,000 chromatographs operating worldwide.¹⁴ Every column replacement requires recalibration. The performance of a column filled with porous solid-phase material, however, depends on subtle details in the pore structure that are difficult to control: pore size, pore size distribution, shape, connectivity, and tortuosity of the pore network, and the distribution of the chemical surface functionalities. Even small deviations caused by production processes or handling can alter separation performance. In addition, the separation of complex compound mixtures requires lengthy and resource-consuming analytical procedures. Shorter, cleaner, and more efficient procedures are desired. Columns in smaller dimensions (e.g., submillimeter) are increasingly becoming important where traditional particle-packing technique require rational design. Such highly specific methods would benefit greatly from precise design of the chromatographic columns' pore structure.

Solution. By precisely controlling the pore structure, it will be possible to manufacture standardized columns. Understanding how pore arrangement influences separation makes it possible to develop targeted stationary phase materials with well-defined pore structure, allowing the optimization of structure-property-performance relationships. This in turn is expected to lead to columns that achieve more precise and reproducible separation while consuming less resources.^{10,15} Fabrication methods being currently developed, especially 3D- and 4D-printing technologies, enable highly precise, reproducible design of fixed or module-like porous structures.^{16–20} They are expected to enable the production of complex, application-specific columns. The additive manufacturing of porous materials has made promising progress in recent years. So far, the highest resolution and complex structures were achieved by light-based 3D printing technologies. Thereby, 3D-printing of polymers is more established as compared to

printing of ceramic structures. While first approaches to print ceramic structures harness established approaches of photopolymer printing while adding silica particles which are sintered into a transparent silica material in a posttreatment,^{21,22} recently, photosol-gel chemistry and the combination of top-down DLP and bottom-up self-assembly techniques at the nanoscale are increasingly investigated.^{16,18,23–26} With optimized printing inks and computer-aided design, it may soon become possible to develop column architectures that were previously out of reach.

Requirements and Recommendation. To improve manufacturing capabilities, new fabrication technologies allowing precise local placement of space over all length scales have to be implemented. Reproducible standards have to be established, and pore architectures have to be translated into robust industrial applications. Characterization methods capable of resolving the details of the pore network arrangements²⁷ need to be further advanced and be combined with material research. Only through systematic validation can robust manufacturing processes be developed and the key parameters identified that ensure high performance and reproducibility.

Catalysis – Harnessing Confinement for New Selectivity

Challenge. Catalysis underpins a large fraction of the global economy: catalytic processes are involved in the manufacture of nearly 90% of chemical products and support industries worth several trillion US dollars, including energy and fuels, bulk and fine chemicals, food production (e.g., fertilizers), and pharmaceuticals. Overall, catalysis is estimated to contribute to products accounting for roughly 30–40% of global GDP. In addition, catalytic processes are involved in ~80% of all manufactured goods, underscoring why advances in catalysis ripple across entire value chains.²⁸ However, catalysis faces pressing challenges: many important reactions remain inefficient, environmentally costly, or inaccessible with today's heterogeneous catalysts. Emerging catalytic approaches, such as electrocatalysis, increasingly rely on porous and nanostructured materials. However, establishing quantitative structure-activity relationships remains challenging due to the complex and often dynamic nature of active sites and porous architectures under operating conditions.^{29–31} Selectivity has to be increased and waste generation has to be minimized while access to bulky, complex molecules that conventional porous catalysts struggle to accommodate has to be engineered. The vast majority of existing heterogeneous catalysts have pore architectures optimized for medium and small molecules. However, many of the molecules that form renewable feedstocks are both bulky and highly functionalized,^{32,33} such as biomolecules, biomass-derivatives, plastic waste, or pharmaceutical intermediates.

Although new classes of nanocatalyst materials continue to emerge,^{34–38} it remains a major challenge to achieve precise, reproducible, and modular control over their internal structural organization across a hierarchy of length scales, from atomic coordination environments to micron-scale architectures. A systematic design approach is still lacking. We do not yet fully understand how pore size, shape, architecture, connectivity, defects or functionalization determine catalytic performance. This is crucial for green chemistry and modern feedstocks as well as for advanced compartmentalized and life-like material systems design. Moreover, controlled confined catalysts are an ideal playground for developing cascade catalytic systems with

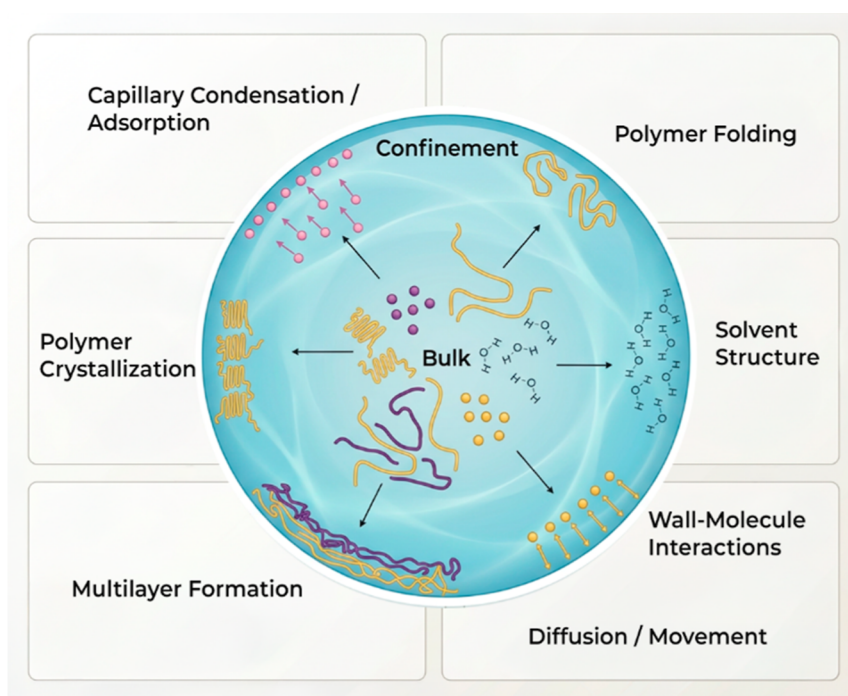


Figure 3. Examples on how confinement influences molecular behavior including transport, dynamics, conformational changes and molecular orientation, nanostructuring on pore surfaces, phase transitions as well as solvent ordering. The scientific content, conceptual organization, and graphical elements of this figure were created by the authors. Artificial intelligence-assisted tools were used exclusively for graphical refinement and aesthetic enhancement.

coupled chemical-chemical, or chemical-biological tandems.^{39–41}

Solution. Nanoconfinement offers a new dimension of control. By restricting the spatial environment around reactants and transition states, it can enhance reaction selectivity and suppress undesired pathways, thereby reducing byproduct formation, energy consumption, and separation demands—key factors for more sustainable chemical processes. In some cases, confinement can even enable reactions that are otherwise inaccessible in bulk environments.^{7,8,42–44} Confinement can improve reactions manifold such as by accelerating the reaction kinetics to produce longer polymers in shorter time,^{45,46} by increasing selectivity in macrocyclization during drug synthesis,^{7,47} and by spatially controlling cascade reactions.^{39,40} A study of CO₂ electroreduction inside confining nanotubes found that the selectivity of methanol synthesis dramatically depends on the nanotube diameter.⁴⁸ By selectively confining reactions to pores or nanocavities, optionally aided by molecular imprinting strategies, aspects of enzymatic catalysis can be mimicked: enzymes control the geometry of substrates, orient reactants precisely, stabilize key intermediates and drive only desired reaction paths.

To tackle the accessibility of bulky and complex molecules, new modularly designed hierarchical porous materials are needed. These would enable the catalytic conversion of large organic intermediates, bioderived building blocks, and even polymer chain-domains where classical microporous materials choke or decompose. Porous materials could also improve chiral control in chemical reactions. This is relevant in the pharmaceutical industry, where two different drug enantiomers may mean the difference between cure or dramatic birth defects such as for thalidomide. Interestingly, in recent work a chiral zeolite yielded enantiomeric enrichment in a test reaction.^{49,50} If nanoconfinement can be combined with

chirality, for example by embedding chiral pore shapes or chiral functional groups within nanoscale cavities, we may approach enzyme-like precision. Furthermore, expanding catalytic capability beyond single-step reactions can integrate multiple, spatially defined catalytic functions to enable combined tandem and cascade reactions. Such integrated architectures hold significant promise for enhancing reaction efficiency, increasing yields, and reducing energy and solvent consumption, e.g. in biomass conversion or in the development of compartmentalized life-like materials.

Requirements and Recommendation. A targeted research strategy on confinement in catalysis should include precision and reproducibility across scales and between different laboratories. Precise and modular hierarchical porous platforms need to be developed that combine molecular access to meso/macropores (2–50 nm)³² and tailored micropores (≈ 0.5 –2 nm) to achieve selectivity, tunable defect density, and surface functionality thereby creating detailed structure–reactivity maps. Data-centric workflows and machine learning can accelerate the identification of optimal pore architectures, while advanced fabrication and in-operando characterization methods can maintain structural fidelity from lab-scale synthesis and prototypes to industrial catalysts. Linking atom-level processing of pore walls and shaping the device will preserve validated pore parameters during scale-up. High-resolution, in-operando, multiscale, multimodal characterization is essential to track active-site states, intermediate lifetimes, and mass transport under realistic conditions, and fuse these data with artificial intelligence(AI)/ machine learning (ML) to extract design rules to understand how confinement controls catalytic reactivity. With this approach, spatially organized multisite catalysts for one-pot tandems/cascades will become accessible and the development of intrinsically chiral porous materials for pharmaceutically

relevant enantioselectivity can be accelerated. Stronger collaboration between academia and industry is essential to bridge the gap from discovery to application. With coordinated support and investment, this field could become a cornerstone of technological innovation and a driving force behind solutions to some of the most pressing social challenges of our time. Together, these efforts will turn nanoconfinement from a qualitative concept into a predictive and scalable technology for designing the next generation of catalysts for sustainable chemical manufacturing, green energy conversion, and precision medicine.

Nanofluidics – Confinement for Emerging Technologies

Challenge. Nanofluidics, the targeted control of transport processes in nanoscale pores, is particularly relevant for energy generation, medicine, and novel devices with memristive behavior, and ion-based computing. A key challenge in the field of nanofluidics is to recover molecules from water or to drastically reduce the high energy consumption of conventional separation processes, which accounts for 10–15% of global energy consumption.²

Solution. Nanofluidics opens conceptually new approaches. The transport of molecules and fluids under confinement enables energy-efficient, fast, and selective transport.^{51,52} Examples include energy harvesting using salt-gradient driven osmosis or overcoming the trade-off between permeability and selectivity in separation. Recently developed resonant osmosis, a method that separates molecules not by size but by the velocity of molecular movement, can be scaled to existing large-scale porous membranes which are currently translated into practice.^{52–55} While still in its infancy, the concept of resonant separation is expected to allow for higher selectivity and reduced energy consumption in separation,⁵² both essential requirements for a circular economy.

In personalized medicine, nanopores are emerging as a key technology. They enable ultrafast, precise, low-cost, and mobile DNA¹¹ sequencing for instance, for cancer diagnostics during surgery. The same principle has been shown for synthetic polymer sequencing.⁵⁶ Translocation of such chains through the nanopore relies on transient molecular deformation and unfolding, and includes changes in the hydration shell and nonequilibrium translocation dynamics (Figure 3). The method is currently being expanded by research on post-translational modifications in proteins, peptides, glycans, and biomolecular interaction analysis, leading to orientation-dependent current signatures.^{11,57–59} This not only broadens its application range but increasingly develops toward a single-molecule confined-state spectroscopy platform and is discussed in the context of chemical data storage.⁶⁰

In parallel, the first innovative approaches are emerging in the field of ionic computing and memristors, in which ions—rather than electrons, as in conventional electronic components—are used as information carriers, similar to the brain.^{61–65} While still at an early stage, this emerging area of iontronics could ultimately yield novel memory and smart-material concepts, particularly if coupled to nanopore-based energy generation for autonomous operation.⁶³

Requirements and Recommendation. Transport processes in confined systems could give rise to a new generation of technologies from energy-efficient separation to precise diagnostics and novel information processing systems. To fully exploit this potential, strong fundamental research (combining experiments with multiscale modeling) and a coordinated

interplay with technology transfer will be essential. Research using highly precise model materials with modularly designed pore space, pore shape, and assembly will be crucial for deepening our fundamental understanding of transport processes as well as the interplay of combined confinement and surface effects. Scaling from single-pore concepts to multipore materials and large-scale membranes will be essential. Current research highlights the significant impact of pore architecture by highly sophisticated model material design.^{66,67} For example, interpore distance or concentration polarization strongly affect the transition from single pore to multipore device performance.^{63,68} Energy-efficient nanopore concepts, such as recently reported resonant osmosis, must be translated into various material strategies and developed toward technology integration. Research orientation should combine curiosity-driven and mission-oriented approaches, with proof-of-concept computer simulations, experiments, and prototypes. Deep tech start-ups will serve as connectors between fundamental research and technology and accelerate innovation, supported by targeted funding for prototyping and industrial collaborations. Structural support through targeted funding programs and the training of a next generation of researchers at the interface between curiosity-driven science and application are indispensable.

Harnessing the Precision of Biological Pores for Emerging Technologies

Challenge. Biological pores are nature's masterpieces for molecular transport — gated, directed, extraordinarily fast, and highly selective. Examples include the potassium channel,⁹ essential for transmitting electrical signals in nerve cells, and aquaporins, which regulate the water balance of cells. Aquaporins can conduct up to 3×10^9 water molecules per subunit per second while blocking ions and other solutes—a combination of speed and selectivity that remains unmatched in technology.⁶⁹

In technical applications, the direct integration of such high-performance biological pores into membranes has been demonstrated in only a few special cases. As one example, aquaporins are used in water filtration. Another example is the use of biological pores in single molecule sensing. Yet, with growing challenges such as water scarcity and sustainable energy supply, there is an urgent need to translate these biological design principles into synthetic, solid-state systems.

Solution. The extraordinary performance of biological pores originates from the precise design of the confined space^{65,70} and the placement of different functional groups. The narrow geometry together with interface properties force molecules into a specific arrangement^{71–73} and shift chemical equilibria.^{74–77} Interactions with functional groups further yield properties and transport efficiencies that are fundamentally different from those in unconfined environments.^{72,78–82} In addition, the functional groups are integrated into compartmentalized systems and regularly renewed in living organisms, keeping the system alive and at high performance.

Transferring the unique capabilities of biological pores to synthetic materials requires a deep understanding of confined space design and fabrication methods capable of producing highly defined confined spaces at the level of individual nanopores, multipore membranes, and compartmentalized system integration.^{40,83–85} These include pore-editing techniques that enable nanopores to be precisely shaped and functionalized using site-specific chemistry with local place-

ment of functional groups or molecular imprinting.^{38,86,87} While nanoscale asymmetric functionalization has been predicted theoretically⁸⁸ to direct transport, experimental implementation is mainly limited to the micrometer scale.^{89,90} Approaches toward nanoscale pore editing remain scarce and are either difficult to scale up^{68,91} or limited in their design flexibility when e.g. using a layer-wise design or an assembly process not allowing to combine individually designed pores into a multipore material. Nanoscale resolution as well as large scale applicability in local pore editing is still a matter of future research. Methods for precise local control^{67,68,91,92} have to be advanced, and concepts for system integration and continuous cleaning or repair are needed to extend service life.

Advanced modeling and simulation can guide this process, predicting efficient pore materials,⁹³ geometries, and arrangements for targeted functions. High-resolution, time-resolved characterization is essential to establish clear structure–function relationships. A notable example of successful translation is zirconium cyclosilicate zeolites (ZS-9), used in medicine to treat hyperkalaemia.⁹⁴ Based on their composition and pore size balancing hydration shell modulation and ion-pore interaction, these microporous materials exhibit a remarkable potassium selectivity close to that of cell membranes. The K⁺ adsorption capacity of ZS-9 is nine times greater than that of organic polymer resins (sodium polystyrenesulfonate) and, compared with resins, ZS-9 is by a factor of over 125 more selective for K⁺ as well allowing it to be separated from Na⁺ or Ca²⁺.⁹⁴

Requirements and Recommendation. Pore editing capabilities must be refined to achieve precise structural and functional control at the level of individual nanopores including the ability to tailor pore geometry, defects, wall composition and functionalization with nanometer accuracy. This will need orthogonal and, at the same time, precise while scalable chemistry and multipore fabrication concepts have to be developed. The design of multipore membranes demands careful control of pore–pore cross-talk and connectivity as well as understanding of the ratio of participating pores to ensure reproducibility at the device scale, when going from a single to the combination of different, precisely designed nanopores.^{68,95} Going toward multipore membranes is, for example, manifested in concentration polarization important in separation but as well in upcoming membrane-based energy conversion.^{63,96} In this endeavour, reproducibility on the individual pore and the multipore assembly level has to be attained and the ratio of participating pores in a multimaterial function needs to be understood. Dynamic behavior needs to be incorporated, and stability at operation ensured. The dynamic adaptation of confinement, such as structural changes triggered by the selective binding of small ions into a channel or a molecule into an enzyme pocket, enhances transport selectivity and speed or catalytic transformation. This is exemplified by the potassium channel, which achieves highly selective and rapid transport demonstrating exquisite control over molecular-scale processes.⁹⁷ Understanding the dynamics in confinement, as well as the interface to supramolecular chemistry, will be an important future research direction, among others, in the context of heavy metal removal or sensing.⁹⁸

Moreover, integrating these porous structures with energy transduction mechanisms such as redox-active components, light, or magnetic-driven actuators, or chemomechanical

systems can facilitate sustained operation beyond thermodynamic equilibrium.^{85,99} Although, redox-active and voltage-gated nanopores have been demonstrated^{64,100,101} and self-powered ionic devices have been proposed,¹⁰² fundamental understanding and integration into complex systems remains a challenge. Achieving this would allow the continuous maintenance of gradients, the selective uptake and release of molecules, and the emergence of autonomous behaviors and complex, compartmentalized material systems. As an example, hierarchical porous structure enabling cascade catalysis between chemical and biological catalysts^{39,40} are a first approach toward compartmentalized material systems. Selective, gated, and directed transport is a key prerequisite to keep molecular gradients active and prevent the system from reaching equilibrium and thus for envisioning so-called “life-like” materials.^{103–106}

Advanced in situ and time-resolved characterization techniques alongside modeling approaches are essential to capture such dynamics and subtle effects such as small pH-changes in situ and in-operando and to guide rational design. At the same time, the wealth of data obtained from these efforts need to become more accessible and enable the development of efficient, accurate machine-learned models for reading-out nanopore signals and detecting sequences and modifications i.e. in proteins and DNA.^{107,108}

Coordinated validation methods such as interlaboratory studies¹⁰⁹ and open-access databases linking pore structures to performance will be key to establishing reliable design rules. Finally, raising awareness and teaching the next generation worldwide will be essential to ensure that the control of confined space becomes a systematic design parameter for new materials, directly addressing the urgent need to develop sustainable solutions for water, energy, and health.

New Technology Concepts by Rethinking Material Properties through Confinement

Challenge. In both biological and synthetic nanopores, the behavior of molecules differs from their bulk behavior (Figure 3). Molecular order and thermodynamics, e.g. phase behavior of fluids such as condensation/evaporation freezing/melting, charge regulation, or crystallization, differ as compared to the unconfined state.^{51,74–76,81} These phenomena are fascinating but often remain poorly understood and are still difficult to harness in a controlled way.

Solution. One important application concerns ion and energy storage. Confinement could help solve a long-standing challenge: the separation of sodium and potassium ions, which is crucial in biology and energy technologies. Likewise, the ultrafast movement of sodium or lithium ions in narrow pores represents a key mechanism for future high-performance battery materials, while selectively choosing the type of ions can significantly modify memristive behavior.^{73,110} As an example, sodium can be intercalated into the small pores of carbon-based materials. As the space is within the length scale of the ion size, the sodium remains liquid inside these pores enabling very high transport rates at high capillary pressures.¹¹⁰ Furthermore, research on fluid intrusion into porous materials demonstrates triboelectric energy harvesting, an effect that still has to be understood. Thereby, nanoporous silicon is shown to be more efficient than powdered porous materials and charge transfer efficiency is enhanced when using conductive nanopores.¹¹¹

In nanopores, water can reach higher densities without crystallizing, while atomic-level and dielectric properties, such as partial charges, hydrogen bonding networks, or local structure possibly differ in confinement, which opens up the possibility of controlling transport processes or reactions under mild conditions.^{67,72,112,113} Confinement also shifts the transition from vapor to liquid, a principle already used in pore size and pore-network characterization,^{114,115} but equally promising for water management/purification, gas separation and storage, or sensing applications.^{116,117} When combined with nanofluidics, new phenomena can emerge, such as faster droplet evaporation at lower temperatures¹¹⁸ due to capillary imbibition and additional evaporation from the fluid-filled porous material. Such phenomena are currently discussed under the topic of hydrovoltaics aiming to harvest energy from confinement and water.^{119–121} Adding ions into the solution further complicates understanding, as evaporation and flow driven local concentrations and osmotic effects become detrimental, affecting imbibition and fluid behavior.^{112,113,122,123} Furthermore, imbibition exerts a strong force on the mesopore walls inducing deformation even in materials such as mesoporous silica monoliths (Vycor), which are expected to be stiff from the bulk material perspective.¹²⁴ Confinement also profoundly affects polymers and biomolecules. The pK_a of acids and polymers shifts inside pores, altering how molecules bind and are released or if enzymes are stable.^{74–76,125} Functional confinement induces significant pK_a shifts, as charge can be regulated by counterion screening, conformational change to increase the distance between charges or by shifting the equilibrium.^{75,76} This has direct implications for drug delivery, protein separation, sensing, and catalysis. Furthermore, an understanding of charge regulation currently remains limited to simple electrolyte solutions and mostly homogeneous nanopore wall functionalization. Confinement facilitates biocatalysis by stabilizing biomolecules, such as proteins, and regulating their local concentration.^{78,126}

There is an opportunity for the design of optical and functional materials and metamaterials. Adsorption and condensation within pores changes optical properties, paving the way for switchable optical, insulating, or even acoustic devices. On the other hand, stability may become a limitation. For example, MOFs with high adsorption capacities usually degrade upon exposure to acidic or basic environments.¹²⁷ Thus, designing a MOF chemistry robust enough to withstand industrial conditions without sacrificing porosity remains a challenge. Finally, confinement can stabilize water droplets¹¹² enabling e.g. technologies for harvesting drinking water from air.

Requirements and Recommendations. To make systematic use of these opportunities, a shift in design principles is required. The size, shape, arrangement, and functionalization of the pores must become the central design parameter. Molecularly imprinted pores made up of self-assembled multifunctional layers and Janus-type asymmetries in pore surfaces are still in their infancy. Characterization techniques must advance to the point where we can effectively “look into the pore” while it is in operation, rather than only analyzing the final products. Developing model materials with well-defined pore structures is essential to unravel fundamental effects, even if these systems are not directly scalable to industrial applications.

Theoretical models including statistical physics-based molecular simulations are indispensable for revealing processes

that are difficult to capture experimentally, such as the distribution of charges or protons within a pore or conformational aspects of synthetic polymers or proteins translocating through the pore. Theory can act as a microscope by quantifying otherwise invisible parameters, and it can serve as a predictive design tool by systematically exploring different pore architectures, materials, as well as solvents. To fulfill these roles, theory must continue to evolve so that it can realistically capture complex systems involving multiple length scales and ideally an entire device.

Digitalization, Automation, and Data-Driven Research—Accelerating Sustainable Innovation

Challenge. The design space for confined structures and synthesis conditions is vast. As a further bottleneck, high-throughput structural characterization often lacks the required resolution, while advanced high-resolution methods are not yet compatible with automation. As a result, the pace of innovation is slower than needed, and reproducible structure–property relationships remain difficult to establish. At the same time, high-throughput numerical approaches are typically related to a high computational demand and strongly rely on high-performance computing (HPC) resources, which in turn hurt sustainability.

Solution. As data-driven materials fabrication relies on the acquisition, analysis, and interpretation of large, high-quality data sets, a seamless connection of fully integrated workflows, robotic synthesis, automation-compatible protocols, high-throughput characterization, and advanced statistical modeling must be achieved.¹²⁸ Data-driven synthesis can transform material construction systematically by combining different building blocks, while robotics-assisted laboratories combine automated synthesis with AI-guided analysis to uncover structure–property relationships.^{128–130} The advances in computing and hardware platforms, including the vision of exascale and quantum computing, promise to significantly expand the accessible scales of materials’ modeling. However, reliable, high-throughput structural characterization often remains a key bottleneck.^{114,131,132} Emerging approaches in statistical image analysis—such as information entropy¹³³ and spatial distribution functions¹³⁴—offer promising pathways to correlate fabrication parameters with resulting structural features, shedding light on heterogeneity across thin film samples. These descriptors can feed into digital twins to predict structure–property relationships at the nanoscale.

Digital twins—created both at the pore level and at the level of integrated systems—can predict material behavior in conjunction with the hierarchical internal confinement structure before prototypes are built and technologies are deployed, reducing risks, costs, and speeding up development. When embedded in machine-learning models tailored to confined systems, they enable in silico screening of material architectures, thereby accelerating discovery and supporting informed decision-making prior to experimental validation. Life-cycle analyses can be embedded early in this process to ensure that factors such as robustness, resilience, and sustainability are taken into account when selecting technological approaches. Machine-learning tools, already used to accelerate materials screening and to evaluate nanopore sensing signals, can be adapted to nanoconfinement to explore large parameter spaces and identify promising candidates efficiently.¹¹⁴ Established industrial processes such as additive manufacturing or roll-to-roll processes can also be integrated

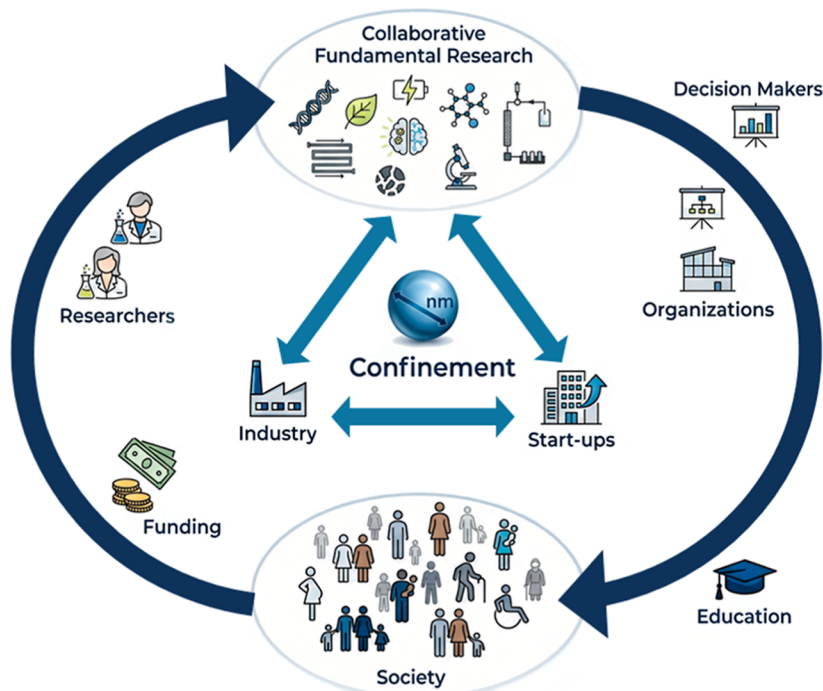


Figure 4. Confinement offers the potential to enable previously unexplored technologies and to accelerate innovation particularly when considering the entire cycle from fundamental interdisciplinary research to technology transfer. Conceptually, confinement can operate across multiple scales, ranging from the molecular level over industrial technologies to society. The authors designed all scientific content, graphical elements, and overall structure of the figure. AI-assisted tools were used solely for color optimization.

into automated workflows,¹²⁹ bridging fundamental research with scalable production.

Requirements and Recommendation. To make these possibilities a reality and to fully explore the vast design space of confinement, open and collaborative infrastructures must be created. These should efficiently combine physics-based modeling, AI/ML algorithms and workflows, as well as digital twins of possible prototypes. Strategic investment into recently developed open-source tools for automation and autonomous synthesis workflows are needed, together with platforms for sharing protocols and data. Service units such as high-performance computing or characterization centers, material libraries, data repositories, and AI toolboxes would allow researchers from different disciplines to access advanced methods and accumulate knowledge collectively. Reliable data management following FAIR principles—findable, accessible, interoperable and reusable—is essential to enable systematic categorization, storage and exchange of results.¹³⁵ Building interdisciplinary communities will be key to accelerating innovation and ensuring that technological development proceeds fast and in a sustainable and coordinated way. Finally, advanced students of all disciplines should be trained to combine their discipline-specific knowledge with AI/ML tools and with tools allowing for automation and automated synthesis to open up new opportunities for interdisciplinary discovery. Educating and training next generations not only leads to the development of new tools and algorithms, but also to a critical evaluation of their applicability and accuracy, in order to avoid “black-box” approaches and promote the development of explainable AI/ML and transferable modeling approaches. Only such an approach will enable a targeted design of nanoconfined materials, and scientifically rigorous, sustainable innovation.

CONCLUSION

Recent advances in the science and engineering of nanoconfinement have underscored its transformative potential as a unifying concept addressing major societal challenges. Confinement at the nanoscale fundamentally alters molecular behavior, enabling enhanced reactivity, improved selectivity and finely tuned transport mechanisms. Research on confinement has shifted from observing confinement effects to rationally engineering confinement at multiple scales, integrating porous frameworks, dynamic architectures, and hybrid organic–inorganic systems. This evolution now includes responsive and reconfigurable pore environments, enabling real-time tuning of transport, catalysis, or separation functions. These properties provide the foundation for next-generation technologies for health, sustainable energy, or water purification, and separation (Figure 4). Developing these could rely on programmable AI-designed confinement or the integration into complex material systems such as hybrid synthetic-biological “life-like” materials.

Despite this promise, significant challenges remain. Above all, confinement as a unifying common design principle has to be strengthened in research and technology. Other central bottlenecks are to fabricate complex nanostructures with high reproducibility across scales from atomic defects over mesoscale connectivity to full device structure, as well as to advance ultrafast and ultrasmall characterization ideally in-operando.

Physics-based computational modeling and artificial intelligence are beginning to bridge some of these gaps, opening the door toward AI-designed confinement. Progress will depend on strong interdisciplinary collaboration integrating material synthesis, in-operando characterization, data science, process engineering, and scaling up. This integration will be of crucial

importance to develop material concepts with increasing precision along all length-scales and down to the molecular level. In addition, the introduction of reproducible standards and the translation of observed function into understanding along all length scales will be highly desirable. Closer interdisciplinary integration between predictive simulation, automated synthesis, and rapid validation is needed to link fundamental science with technological readiness. Importantly, the pace of translating fundamental insights and natural design principles into scalable, nature-inspired, robust, and economically viable new technologies has to be accelerated e.g. by close cooperation with industry partners and by funding start-ups.

To fully capitalize on these opportunities, decision makers should prioritize investment in both fundamental and translational research, ensuring that highly original fundamental science advances rapidly while coupling it to real-world problem solving, thereby accelerating the pace of innovation. At the same time, the training of highly qualified researchers must evolve beyond just the use of the wealth of currently developing computational tools and experimental procedures: new generations need sound disciplinary knowledge and conceptual understanding of confinement effects, but also problem-solving and data handling skills, systems thinking and experience in interdisciplinary collaboration. Embedding innovation-driven case studies into disciplinary curricula enhances diversity while strengthening both solid disciplinary knowledge and the ability to translate knowledge into applied technology.

Finally, while physical confinement at the nanoscale offers a wealth of technological opportunities, beyond science another meaning of the word 'confinement' carries social and cultural implications. Experiences from recent global crises remind us that social confinement of a person during a pandemic lockdown can restrict openness, reduce cultural exchange, and increase polarized opinions. Yet, the social confinement has also catalyzed positive changes: strengthening the bonds among family, friends, and professional colleagues, encouraging new modes of communication such as video calls, and reducing the carbon footprint by reduced travel. Acknowledging both limitations and advantages, and finding the right and case-specific balance between confinement and open space is an important topic to be considered. This underlines the importance of designing technologies that are not only efficient and sustainable but also inclusive and human-centered.

In conclusion, advancing nanoconfinement science provides a unique opportunity to reshape how we design materials and processes to confront pressing global challenges. With continued support for research, education, innovation, and collaboration, and with awareness of the broader societal meaning of confinement, confinement as unifying design principle will deliver clear benefits for science, technology, and society.

AUTHOR INFORMATION

Corresponding Authors

A. Andrieu-Brunsen – Ernst-Berl Institut Für Technische und Makromolekulare Chemie, Technische Universität Darmstadt, Darmstadt 64287, Germany; orcid.org/0000-0002-3850-3047; Email: annette.andrieu-brunsen@tu-darmstadt.de

O. Azzaroni – Instituto de Investigaciones Físicoquímicas Teóricas y Aplicadas (INIFTA), CONICET, and Departamento de Química, Facultad de Ciencias Exactas, Universidad Nacional de La Plata, La Plata 1900 Buenos Aires, Argentina; orcid.org/0000-0002-5098-0612; Email: omarazzaroni@quimica.unlp.edu.ar

G. J. A. A. Soler-Illia – Instituto de Nanosistemas, Escuela de Bio y Nanotecnologías, (INS-EBYN-UNSAM-CONICET), San Martín 1650, Argentina; orcid.org/0000-0001-9984-3806; Email: gsoler-illia@unsam.edu.ar

Authors

H. Binyaminov – Colloid Chemistry Department, Max Planck Institute of Colloids and Interfaces, Potsdam 14476, Germany

A. Danil de Namor – School of Chemistry & Chemical Engineering, FEPS, University of Surrey, Surrey GU2 7XH, U.K.

M. Fyta – Computational Biotechnology, RWTH Aachen University, Aachen 52074, Germany; Center for Computational Life Sciences, RWTH Aachen University, Aachen 52074, Germany; orcid.org/0000-0002-5425-7907

J. García-Martínez – Laboratorio de Nanotecnología Molecular, Departamento de Química Inorgánica, Universidad de Alicante, Alicante 03690, Spain; orcid.org/0000-0002-7089-4973

S. Guldin – Technical University of Munich, School of Life Sciences, Freising, Germany, Singapore 138602, Singapore; School of Materials Science and Engineering, Nanyang Technical University, Singapore 639798, Singapore; Department of Chemical Engineering, University College London, London WC1E 7JE, U.K.

S. Howorka – Department of Chemistry & Institute of Structural Molecular Biology, University College London, London WC1H 0AJ, U.K.; orcid.org/0000-0002-6527-2846

S. Lamotte – Analytical and Material Science, BASF SE, Ludwigshafen am Rhein 67056, Germany

S. G. Lemay – Huygens-Kamerlingh Onnes Laboratory, Leiden Institute of Physics Leiden University, Niels Bohrweg 2 2333 CA, The Netherlands; orcid.org/0000-0002-0404-3169

B. V. Lotsch – Max Planck Institute for Solid State Research, Stuttgart 70569, Germany; orcid.org/0000-0002-3094-303X

S. Magdassi – Institute of Chemistry, the Hebrew University of Jerusalem, Jerusalem 91904, Israel; orcid.org/0000-0002-6794-0553

K. Nakanishi – Institute of Materials and Systems for Sustainability, Nagoya University, Nagoya 464-8601, Japan; Program-Specific Professor, Institute for Integrated Cell-Materials Sciences (iCeMS), Kyoto University Institute of Advanced Study, Kyoto University, Kyoto 606-8501, Japan

C. Plueg – Susionity Commercial GmbH, Industriepark Hoechst G875, Frankfurt D-65929, Germany

S. Polarz – Leibniz-University Hannover Chair for Inorganic Chemistry: Molecular and Material Science, Hannover 30167, Germany; orcid.org/0000-0003-1651-4906

L. Pozzo – Department of Chemical Engineering, Molecular Engineering and Sciences Institute, and Department of Human Centered Design and Engineering, University of Washington, Seattle, Washington 98195-1750, United States; orcid.org/0000-0001-7104-9061

- M. Rafti** – Instituto de Investigaciones Fisicoquímicas Teóricas y Aplicadas (INIFTA), CONICET, and Departamento de Química, Facultad de Ciencias Exactas, Universidad Nacional de La Plata, La Plata 1900 Buenos Aires, Argentina; orcid.org/0000-0003-3393-358X
- M. Rehahn** – Ernst-Berl Institut Für Technische und Makromolekulare Chemie, Technische Universität Darmstadt, Darmstadt 64287, Germany
- A. G. Roth** – Nanostone Water GmbH, Halberstadt 38820, Germany
- C. Sanchez** – Institute for Advanced Study, University of Strasbourg, Strasbourg 67083, France; Laboratoire de Chimie de la Matière Condensée de Paris, Sorbonne Université, Paris Cedex 05 75252, France; orcid.org/0000-0002-6426-4844
- D. A. Scherlis** – Departamento de Química Inorgánica, Analítica y Química Física/INQUIMAE, Facultad de Ciencias Exactas y Naturales, Universidad de Buenos Aires, Buenos Aires C1428EHA, Argentina; orcid.org/0000-0002-0588-287X
- I. Szleifer** – Department of Biomedical Engineering and Department of Chemistry, Northwestern University, Evanston, Illinois 60208, United States; orcid.org/0000-0002-8708-0335
- K. Tschulik** – Lehrstuhl Für Analytische Chemie, Ruhr-Universität Bochum, Universitätsstr, Bochum 44801, Germany; orcid.org/0000-0001-7637-4082
- M. Thommes** – Department of Chemical and Biological Engineering, Friedrich-Alexander-University Erlangen-Nürnberg, Erlangen 91058, Germany; orcid.org/0000-0002-3702-4976
- E. Toimil-Molares** – Materials Research Department, GSI Helmholtz Centre for Heavy Ion Research and Materials and Geosciences Department, Technical University of Darmstadt, Darmstadt 64287, Germany

Complete contact information is available at:
<https://pubs.acs.org/10.1021/jacsau.6c00663>

Notes

The authors declare no competing financial interest.

ACKNOWLEDGMENTS

We gratefully acknowledge Markus Antonietti (Max Planck Institute of Colloids and Interfaces, Germany), Lyderic Bocquet (CNRS and Professor of Physics at ENS Ecole Normale Supérieure, Paris, France) and Christian Kuttner for fruitful discussions and support. We thank Dirk Hans und Hannes Schlender, scienceRELATIONS–Wissenschaftskommunikation for moderating our scoping workshop and for supporting us in translating science into understandable language. We thank Lisa Balonier, Michael Zoppelt (research group A.A.-B., Macromolecular Chemistry-Smart Membranes, Technische Universität Darmstadt, Germany) supporting the organization and documentation of the Scoping Workshop. We thank Tobias Hoffmann (research group A.A.-B., Macromolecular Chemistry-Smart Membranes, Technische Universität Darmstadt, Germany) and M. Lorena Cortez (research group O.A., INIFTA, La Plata, Argentina) for the design of the Figures in this manuscript. The authors used ChatGPT, NotebookLM, and Adobe Firefly solely to assist with graphical refinement of selected figures, including color optimization, visual enhancement, and icon redesign. All scientific content,

figure concepts, layouts, graphical elements, interpretations, and conclusions were conceived, created, verified, and approved by the authors. The AI tools were not used to generate scientific data, results, analyses, or conclusions. We gratefully acknowledge the Volkswagen Foundation for funding the Scoping Workshop “Nanoconfinement in Chemistry”, that provided the basis for this Perspective Article. J.G.M. thanks(9D736)the funding received from the Spanish Ministry of Science, Grant PID2021-1287610B-C21 by MCIN/AEI/10.13039/501100011033 through “ERDF A way of making Europe,” the Generalitat Valenciana through CIPROM/2023/2, and the Advanced Materials Program, and was supported by MCIN with the European Union NextGenerationEU (PRTR-C17. I1) and Generalitat Valenciana. G.J.A.A.S.-I. acknowledges Agencia Nacional de Promoción Científica y Tecnológica (PICT 2020-03130, Proyectos Federales de Alto Impacto 2023 #87), UNSAM (UNSAM Investiga 80020250100112SM) and AFOSR (AWARD NO. FA9550-24-1-0209) for funding.

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