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Bridging the Art and Science: A Symposium Honoring Prof. Luis M. Liz-Marzán for the Dong Qin ACS Award in Nanochemistry

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Abstract:

This Nano Focus article summarizes the symposium honoring the inaugural Dong Qin ACS Award in Nanochemistry at the ACS Spring 2026 meeting. The event celebrated the first recipient, Prof. Luis M. Liz-Marzán, and honored the legacy of Prof. Dong Qin. Key themes included data-driven and machine-learning-assisted synthesis, the engineering of chiral and asymmetric nanostructures for biomedical sensing, therapeutic delivery at the nano-bio interface, and high-throughput single-particle characterization techniques. Ultimately, the symposium showcased a future in which nanochemistry is increasingly automated, predictive, and biologically integrated.

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The inaugural Dong Qin ACS Award in Nanochemistry symposium, held during the ACS Spring 2026 meeting, marked a historic moment for the Division of Colloid and Surface Chemistry. The event celebrated the extraordinary career of Prof. Luis M. Liz-Marzán, the first recipient of the award, while honoring the enduring legacy of the late Prof. Dong Qin (1967–2023). Established in 2024, the Dong Qin ACS Award commemorates Prof. Qin, a visionary at the Georgia Institute of Technology known for her pioneering work in the colloidal synthesis and functionalization of noble-metal nanocrystals. Her colleagues and friends recall a scientist who transformed the "art" of nanocrystal growth into a quantitative science through innovative *in situ* techniques. Beyond the lab, the symposium reflected her "loud, boisterous, and joyful" energy and her dedication to mentoring and community. The selection of Prof. Luis M. Liz-Marzán (CIC biomaGUNE and Universidade de Vigo) as the first awardee perfectly encapsulates the award's purpose: recognizing creative and impactful research in nanochemistry. Prof. Liz-Marzán's leadership in the colloidal synthesis of metal nanoparticles has provided the community with the tools to tailor optical properties and self-assembly at the nanoscale.

This Nano Focus article summarizes the technical advancements presented at the 2026 Dong Qin ACS Award Symposium. The event underscored the evolution of nanochemistry from an empirical art into a quantitative, predictive science. Key themes include the transition toward data-driven and machine-learning-assisted synthesis, the exploration of chiral and asymmetric nanostructures for biomedical sensing, and the development of high-throughput single-particle characterization techniques.

1. Advanced Synthesis: From Data-Driven Design to Symmetry Breaking

The core technical sessions of the symposium masterfully illustrated a profound, paradigm-shifting evolution in the field: the definitive transition from empirical "trial-and-error" colloidal recipes toward highly predictive, automated, and tightly controlled kinetic methodologies. Historically, as noted by contemporaries like Peidong Yang, metal nanocrystal growth in solution has long been treated more as a qualitative art than a quantitative science due to the immense difficulty of capturing atomic-level nucleation and growth dynamics *in situ*.[1] The pioneering work of the late Prof. Dong Qin in developing in situ techniques was central to turning this empirical art of nanocrystal growth into a quantitative discipline. The presentations in this section built directly upon that foundational philosophy, showcasing how modern nanochemistry now couples advanced

computational insights with exogenous physical stimuli to orchestrate crystal growth with unprecedented atomic precision.

1.1 Data-Driven Nanocrystal Design and Machine Learning

A premier example of this digital transformation was presented by **Prof. Chad Mirkin**, who detailed a powerful, data-driven framework designed to bypass classic experimental bottlenecks. Nanoparticles of high-index facets possess an abundance of low-coordination surface atoms and high reactivity, offering exceptional catalytic, optical, and electronic properties. However, these high-energy surfaces are inherently thermodynamically unstable and tend to naturally evolve into lower-energy, low-index ones, making their targeted synthesis an enduring challenge. Mirkin's group tackled this challenge by manipulating surface energies through sophisticated alloying and dealloying processes, where guest atoms are selectively incorporated at the surface to stabilize complex high-index architectures. Because the sheer number of host-guest elemental combinations is too vast for manual, trial-and-error experimental screening, they integrated high-throughput density functional theory (DFT) calculations with machine learning (ML) models. This computational engine rapidly evaluates surface energies and predicts the exact stabilization conditions required to yield targeted morphologies. By validating these insights with high-throughput synthesis and screening, the strategy successfully uncovered pristine high-index facet nanoparticles—including tetrahexahedron ({210} facets), hexoctahedron ({421} facets), and even high-entropy nanoparticles composed of up to seven distinct elements.[2] This methodology effectively transforms nanomaterials design from a discovery-based effort into a deliberate engineering science.

1.2 Kinetic Control, Twinning Defects, and Spontaneous Symmetry Breaking

Providing an exploration of fundamental reaction and growth kinetics, **Prof. Younan Xia** discussed the ubiquitous and spontaneous phenomenon of symmetry breaking in colloidal systems. Spontaneous symmetry breaking occurs when a system is subjected to microscopic variations in size or subtle perturbations in thermodynamic parameters. Xia demonstrated that these phenomena can be deliberately harnessed and directed by balancing the rate of atom deposition against surface diffusion, or by intentionally introducing structural twin defects into the initial seed crystals. Using palladium (Pd) as a model system, Xia's group illustrated how controlling the precise kinetics of

Pd atom deposition onto symmetric Pd cubic seeds forces the system away from isotropic growth, resulting in highly anisotropic structures like Pd bars, rods, and tripods.[3, 4] Furthermore, they demonstrated that symmetry breaking can be combined with galvanic replacement and co-reduction to generate asymmetric, hollow nanostructures such as nanoboxes and nanocages.[5] These highly anisotropic particles exhibit exotic optical, electronic, and catalytic signatures completely absent in their highly symmetric counterparts, opening advanced frontiers for sensing and structural catalysis.

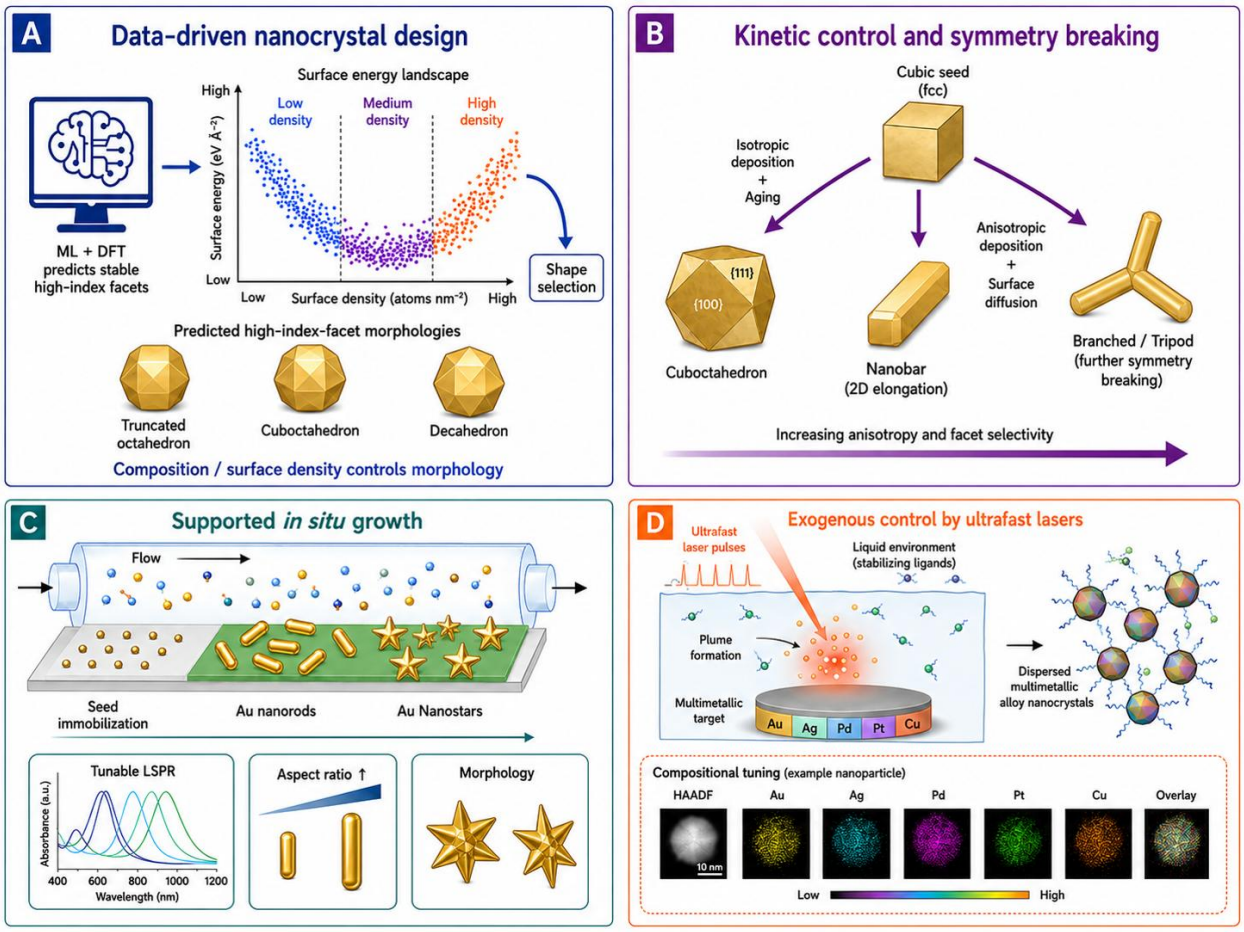

Figure 1. Advanced Synthesis: From Data-Driven Design to Symmetry Breaking. (A) Data-driven/ML-assisted design of high-index-facet nanoparticles, including a workflow linking DFT, surface-energy prediction, and experimental validation.[2] (B) Kinetic symmetry breaking in Pd nanocrystals, showing the transition from cubic seeds to Pd nanorods, or tripods.[3] (C) In situ growth of supported Au nanorods in microfluidic channels, highlighting direct surface integration.[7] (D) Exogenous light or ultrafast-laser-assisted processing of multimetallic colloids.[9]

1.3 Substrate-Mediated Symmetry Breaking and Directed In Situ Growth

Expanding the concept of symmetry breaking from colloidal solution chemistry to solid-state boundaries, **Prof. Svetlana Neretina** addressed the challenges of synthesizing asymmetric plasmonic nanostructures. While symmetric plasmonic shapes are readily accessible via bulk solution methods, creating highly asymmetric shapes with precise substrate orientations remains difficult. Neretina's group successfully broke mirror symmetry during crystal growth by using the underlying substrate itself as a physical template (or confinement). Substrate-bound asymmetric structures, including multi-component Janus nanoparticles, were synthesized by precisely dictating the interfacial growth conditions.[6] These uniquely oriented configurations induce powerful local electric field enhancements and strong circular dichroism, which can be directly exploited in chip-based photonics and molecular sensing.

Complementing this theme of surface-bound architectures, **Prof. Leonardo Scarabelli** introduced a patterned, *in situ* growth paradigm designed to bridge the historical quality gap between liquid-phase colloidal chemistry and solid-state nanofabrication. Traditionally, integration of plasmonic structures onto surfaces relies on post-synthetic colloidal assembly, which frequently suffers from spatial disorder and ligand contamination. Scarabelli's approach chemically constructs nanostructures from the bottom up at pre-determined lithographic locations directly on the substrate. High-yield growth of highly anisotropic plasmonic structures was achieved by combining microfluidics with localized electrochemical and electromagnetic potentials.[7] This approach circumvents the need for independent colloidal synthesis and self-assembly entirely, while maintaining stringent control over crystallography, shape morphology, and surface chemistry. The resulting plasmonic metasurfaces exhibit remarkably narrow collective resonances, providing a crucial stepping stone toward dynamic, chemically active metamaterials.

1.4 Exogenous Control: Photocatalytic and Ultrafast Laser Processing

The final dimension of modern synthetic control highlighted at the symposium revolved around the use of exogenous energy fields—specifically light—to dictate reaction pathways that are completely inaccessible through conventional thermal heating. **Prof. Jill Millstone** detailed the extensive challenges of simultaneously controlling stoichiometry and atomic arrangements in multimetallic nanoparticles, particularly when the constituent metal precursors possess vastly

different intrinsic reduction kinetics. To bypass these thermodynamic limitations, Millstone's group utilized exogenous factors including continuous light illumination and time-dependent precursor addition.[8] They demonstrated that targeted photo-illumination can drive the reduction of mixed metal precursors under ambient thermal conditions, enabling the synthesis of highly uniform, complex alloy and core-shell architectures with tailored properties for energy conversion.

Taking photo-mediated processing to the ultimate temporal limit, **Prof. Andrés Guerrero-Martínez** demonstrated the utility of combining ultrafast laser technologies with colloidal chemistry. While conventional nanosecond laser pulses often cause destructive fragmentation of nanostructures, femtosecond laser pulses interact with electron dynamics on a timescale that permits controlled surface melting and precise size tuning without destroying the particle core. Extending these ultrafast protocols to multimetallic colloidal systems allows for the clean formation of nanoalloys with highly tunable compositions.[9] This precise laser processing provides structural and electronic stabilities that surpass those achieved by purely thermal pathways, offering a robust foundation for designing next-generation plasmonic devices and robust catalysts.

2. The Nano-Bio Interface and Therapeutic Delivery

A significant portion of the symposium focused intensely on the nano-bio interface, illuminating how precisely engineered nanostructures interact with, probe, and navigate complex biological systems. Moving beyond traditional toxicity assessments, modern nanochemistry has treated the biological environment as a dynamic, reciprocal interface where cellular machinery and synthetic nanomaterials actively communicate. This session emphasized that achieving reproducible clinical and diagnostic outcomes requires a molecular-level mastery of surface chemistry, structural scaffolding, and structural rigidity. The presentations detailed a profound evolution from simple, non-specific payload carriers to highly sophisticated, multi-dimensional architectures that seamlessly integrate with living organisms.

2.1 Versatile Biomaterial Platforms for Complex Biologics Delivery

Prof. Frank Caruso introduced a highly versatile, biomaterial-based nanoparticle platform engineered to address the critical hurdles of modern pharmacology. While the global deployment of lipid nanoparticles encapsulating mRNA to combat COVID-19 firmly validated the transformative potential of nanotechnology in medicine, traditional encapsulation techniques

remain highly inflexible, requiring custom, case-by-case chemical formulations tailored to specific therapeutic molecules. To bypass this empirical bottleneck, Caruso's group developed an adaptable, modular assembly approach that allows structurally distinct therapeutic classes—ranging from functional small molecule drugs and rigid proteins to delicate genetic payloads like siRNA and mRNA—to be seamlessly integrated into a single, cohesive nanoparticle archetype.[10] It is worth highlighting that this supramolecular assembly technique relies on non-destructive, non-covalent stabilizing interactions that preserve the native conformation and intrinsic biological activity of the fragile payloads. Upon cellular internalization, the biomaterial vector is engineered to respond directly to the intracellular milieu, undergoing triggered, controlled degradation to release the intact therapeutic cargo precisely at its subcellular destination. This strategy shifts the delivery paradigm away from bespoke formulation chemistry toward a universal, plug-and-play engineering platform.

2.2 Structural Scaffolding: DNA and Protein-Templated Self-Assembly

Shifting the focus toward spatial orchestration at the sub-10 nm scale, **Prof. Qiangbin Wang** and **Prof. David Ginger** highlighted the use of programmable biological macromolecules as templates to direct the rational assembly of inorganic functional nanomaterials. Wang addressed the inherent limitations of top-down fabrication techniques, noting that conventional lithography lacks the processing resolution required to manipulate matter at the true nanoscale, thereby hindering our ability to fine-tune collective material properties. His group leverages the predictable base pairing of DNA and the precise spatial folding of protein templates to direct the bottom-up fabrication of highly ordered, multidimensional architectures.[11, 12] Because the collective optoelectronic and physical signatures of these assemblies depend on the precise quantity, identity, and spatial coordinates of their constituent building blocks, these biomolecular frameworks provide a level of structural control that was previously impossible.

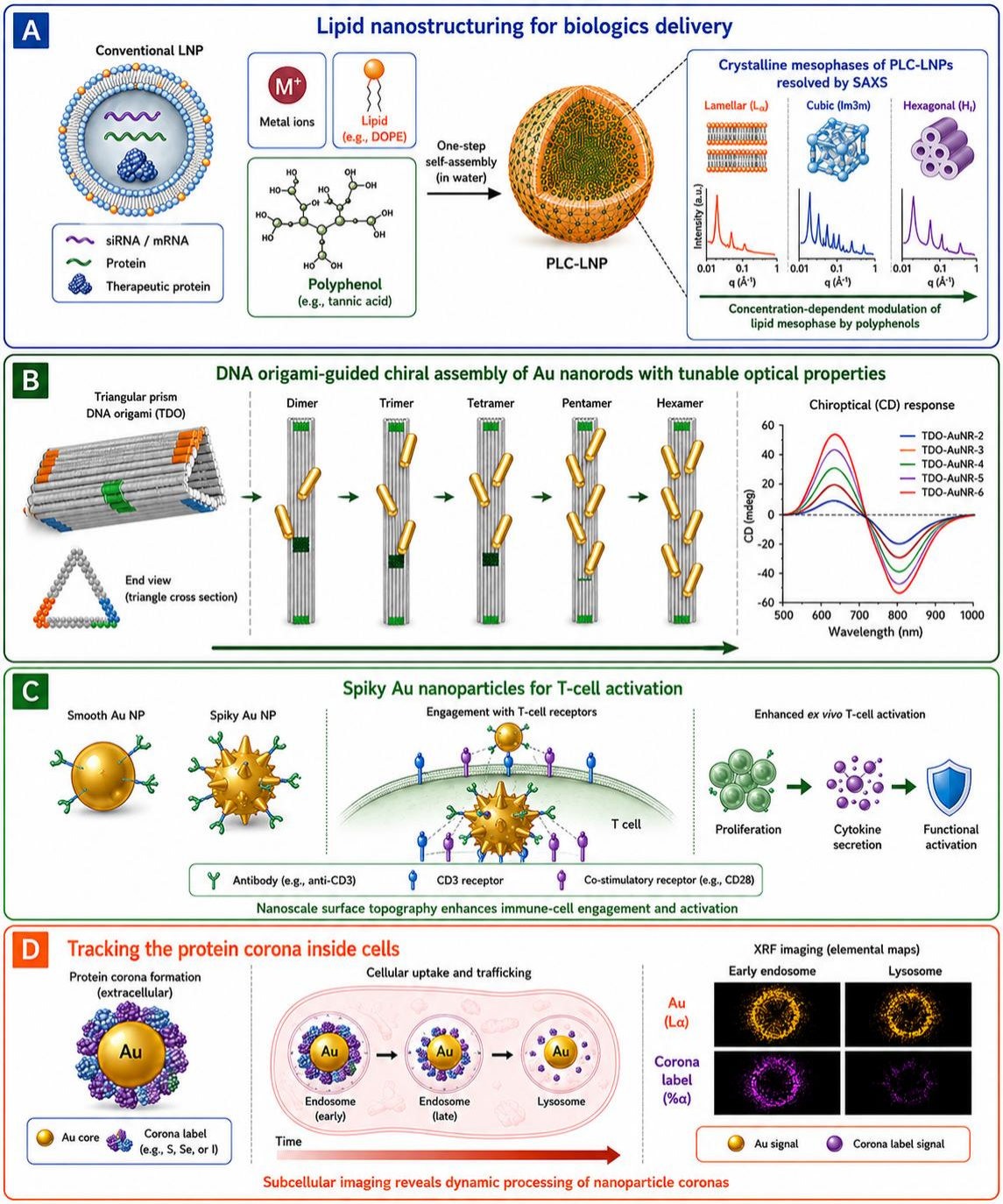

Figure 2. The Nano-Bio Interface and Therapeutic Delivery. (A) Biomaterial/lipid nanoparticle platform with crystalline mesophases for complex biologics delivery.[10] (B) DNA-origami-guided helical assembly of Au nanorods with tailored optical chirality.[11] (C) Spiky or star-like gold nanoparticles for enhanced biomolecular or T-cell interactions.[14] (D) Synchrotron/nanofocused X-ray fluorescence mapping of nanoparticle fate in biological environments.[16]

Ginger's presentation expanded on this theme by showing how these bio-templated nanostructures act as exceptionally sensitive probes of the assembly process itself. Focusing on architectures derived from *de novo* designed protein fibers and highly organized DNA-based voxel frameworks, Ginger's group studies the complex chiroptical effects—such as powerful circular dichroism in optical scattering—that emerge when plasmonic nanoparticles are arranged in asymmetric, helical configurations. To unravel the structure-function relationships governing these soft-hard hybrid materials, Ginger introduced an advanced computational workflow that integrates variational autoencoders (VAEs) utilizing a shared latent space. This machine learning framework allows researchers to extract and reconstruct precise nanoscale structural parameters using exclusively far-field optical spectra embedded with polarization data.[13] By coupling experimental biopolymer templating with deep learning, this methodology establishes a direct, predictive bridge between macroscopic optical behavior and sub-nanometer structural organization.

2.3 Geometric Design for Advanced Biomolecule Delivery

Further bridging the gap between rigorous shape control and practical medical applications, Prof. **Teri Odom** detailed her group's approach to manipulating the structural features of gold (Au) nanocrystals. She focused on the rational design of Au nanostars, spiky nanoparticles, and related structures displaying complex global and local anisotropic features. By thoroughly mapping the growth mechanisms of these branched nanomaterials, her group has established robust methods to tune their localized architectures for high-efficiency biomedical applications.[14, 15] This precise geometric control over spiky and star-like shapes provides a unique platform to optimize the vehicle interface for targeted encapsulation and delivery of fragile biomolecules, such as nucleic acids and proteins, demonstrating how tailored physical anisotropy can directly overcome transport barriers encountered in living systems.

2.4 Synchrotron Fate Mapping and Life Science Assays

Bringing advanced physical characterization directly into the realm of medicine, **Prof. Wolfgang Parak** discussed how fundamental materials science can provide the crucial analytical toolkits and assays required to solve complex biological questions. Parak emphasized that

evaluating the clinical viability of candidate nanomedicines requires a deep understanding of their long-term *in vivo* journey, specifically how they degrade, clear, and distribute across various tissues. To achieve this, his group integrated custom-synthesized colloidal nanomaterials with high-brilliance synchrotron radiation techniques.[16, 17] This combination allows for ultra-sensitive, element-specific mapping and real-time degradation tracking within complex biological matrices. These synchrotron-assisted analytical methods offer deep insights into the exact chemical transformation, elemental fate, and structural stability of nanoparticles over extended periods, providing a rigorous, quantitative framework for designing safer and more effective therapeutic vectors.

2.5 Interfacial Ligand Chemistry and High-Precision Nanothermometry

Prof. Catherine Murphy provided a comprehensive "then and now" look at gold (Au) nanorod synthesis and functionalization, emphasizing the importance of the immediate surface layer. While the early days of nanochemistry focused primarily on controlling the core size and shape of crystals viewed via transmission electron microscopy (TEM), the past fifteen years have shifted toward mapping the precise molecular landscape at the fluid-nanocrystal interface. In the classic seed-mediated synthesis of Au nanorods using cetyltrimethylammonium bromide (CTAB) as surfactant, it is well established that the final product features distinct {111}, {100}, or {110} facets protected by a dense, interdigitated CTAB bilayer. Murphy detailed her group's latest breakthroughs in understanding how this dynamic ligand layer can be manipulated to control the localized surface chemistry and subsequent biological interactions of the nanorod. Specifically, they explored the thermodynamic displacement of the native, cytotoxic CTAB bilayer by various functionalized, thiolated polyethylene glycol (PEG) molecules, evaluating how this ligand exchange affects colloidal stability and cellular uptake. Furthermore, Murphy highlighted the application of these highly optimized Au nanorods as non-invasive "nanothermometers" within active biological systems.[18] In these diagnostic applications, the integrity and composition of the surface ligand shell are absolutely critical; subtle changes in ligand packing directly dictate the particle's photothermal performance, biological safety, and sensing accuracy. Her presentation emphasizes a fundamental principle of the discipline: at the nano-bio interface, the surface ligand chemistry determines the identity of the material.

3. Chiral Nanochemistry and Sensing

The engineering and manifestation of chirality at the nanoscale emerged as one of the most vibrant and technologically promising frontiers discussed at the symposium. Moving far beyond the classical understanding of molecular asymmetry, the presentations at this symposium demonstrated that nanoscale chirality can induce massive chiroptical effects—such as giant ellipticity, sharp circular dichroism (CD) peaks, and intense circularly polarized light emission (CPLE)—that are unattainable with binary molecular systems alone. By blending precise colloidal synthesis with structural biology concepts, researchers are now capable of forcing inorganic crystals into non-centrosymmetric configurations. This enables the creation of highly specialized nanomaterials tailored for enantioselective catalysis, polarization optics, and advanced biomedical diagnostics. The presentations collectively underscored how manipulating spatial handedness allows for incredibly specific molecular interactions, particularly at the interfaces of complex disease biomarkers.

3.1 Inscribing Asymmetry: Chiral Templating via Inorganic Molds

Addressing the fundamental synthetic challenges of this field, **Prof. Ki Tae Nam** presented a powerful and highly reliable strategy for the fabrication of chiral inorganic nanomaterials. Achieving high enantiomeric excess and precise morphology control in metal nanoparticles remains a significant obstacle when relying solely on traditional solution-phase chemistry. Nam's group pioneered an elegant, top-down-inspired colloidal approach using custom-engineered chiral silica molds. These sophisticated molds are fabricated via a surfactant-templated co-assembly process that leads to the formation of highly ordered, topologically chiral pores. By infiltrating these asymmetric pores with noble metal precursors (including silver, palladium, and platinum) and subsequently executing a controlled reduction, the growing metal crystals are forced to mirror the exact spatial handedness and structural morphology dictated by the underlying silica framework.[19] Nam demonstrated that the overall size, shape, and magnitude of optical activity of the resulting metal nanoparticles can be continuously tuned by varying the structural properties of the starting silica template and the chemical reduction conditions. The resulting materials display intense optical activity, opening robust new avenues for enantioselective sensing and asymmetric heterogeneous catalysis.

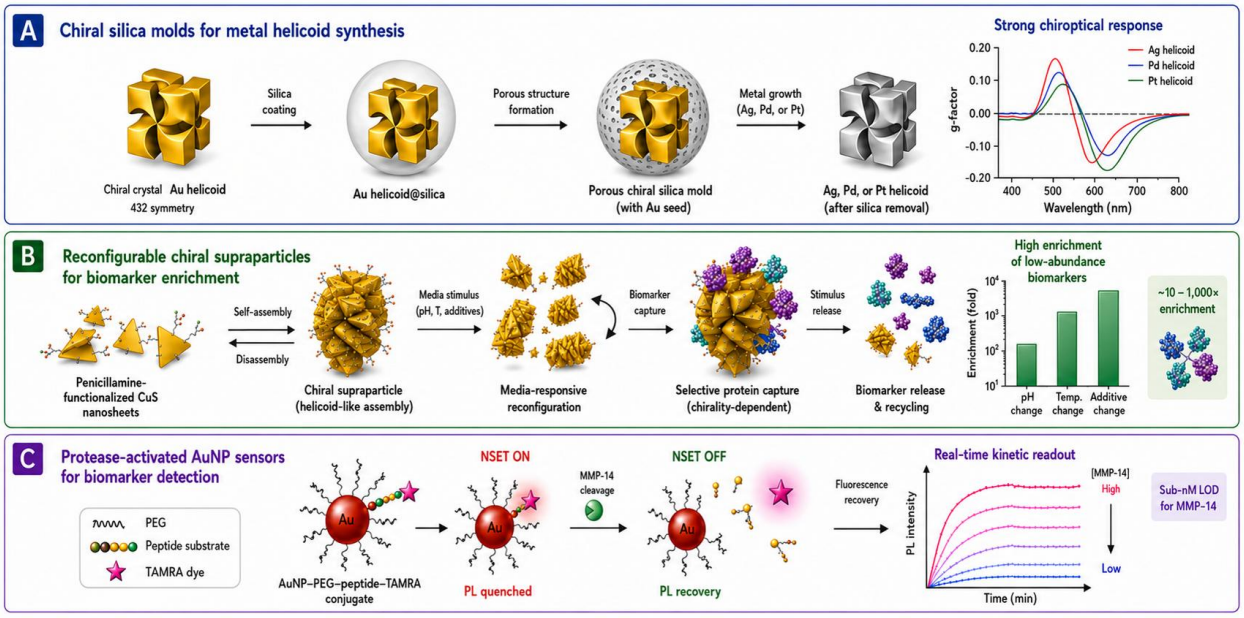

Figure 3. Chiral nanochemistry and optical sensing. (A) Chiral/helicoid gold nanoparticles or conformal nanogap-engineered helicoid structures displaying strong chiroptical response.[19] (B) Reconfigurable chiral nanoassemblies or chiral "transformer" particles for selective biomarker enrichment.[20] (C) Au nanoparticle bioconjugates for optical sensing at the biointerface.[21]

3.2 Giant Ellipticity and Selective Biomolecular Recognition

Taking a multi-scale, biomimetic approach to nanoscale asymmetry, **Prof. Nicholas Kotov** detailed the synthesis, unique properties, and biomedical applications of complex chiral nanostructures. Kotov emphasized that these advanced materials could display giant chiroptical ellipticity that dwarfs the optical responses seen in natural molecular systems, making them exceptional candidates for next-generation biosensing platforms. A focus of his presentation revolved around the engineering of "chiral hedgehog particles"—highly structured, spiky nanoparticles designed with a specific spatial handedness.[20] The primary objective of this work is to leverage these intricate topologies to achieve highly selective, lock-and-key binding interactions with targeted biological counterparts *in vivo*. Specifically, Kotov highlighted the immense promise of utilizing these chiral hedgehog particles for early-stage cancer detection, where their unique shape and handedness allow them to selectively bind to specific malignant cellular membranes or biomarkers. Looking toward the future, his group is expanding this platform to investigate more deeply the fundamental rules governing complex biological self-assembly, to construct high-

performance CPLE-based biological sensors, and to implement real-time holographic imaging for advanced biomedical diagnostics.

3.3 Optically Addressable Bio-Conjugates and Proteolytic Kinetics

Shifting the focus toward ultra-sensitive, real-time diagnostic sensing at the nano-bio interface, **Prof. Hedi Mattoussi** reported on the development of highly optimized Au nanoparticle/peptide conjugates designed to map enzyme dynamics. It is well-established that plasmonic nanostructures interact strongly with proximal fluorophores, acting as highly efficient energy acceptors that quench the emission of nearby organic dyes. Mattoussi's group exploited this phenomenon to engineer a robust, optically addressable sensing platform specifically tailored to quantify the catalytic efficiency of human matrix metalloproteinase-14 (MMP-14), an important enzyme and established biomarker associated with cancer progression and tumor metastasis. The architecture of the sensor relies on clean colloidal Au nanoparticles heavily functionalized with dye-labeled peptide sequences containing specific cleavage sites for the target protease. When these conjugates are introduced to an environment containing active MMP-14, the enzyme systematically cleaves the surface-tethered peptides. As the fragments break away, the dye molecules diffuse away from the plasmonic surface, triggering a time-dependent, quantitative recovery of the fluorescence emission. By tracking these emission kinetics in real time, Mattoussi's group achieved exceptional sub-nanomolar detection limits for the target enzyme.[21] Mattoussi also highlighted how his group incorporated conceptual rationales that account for nanoparticle size, reduced Brownian diffusion, and steric crowding on the dense nanoparticle surface to accurately model the proteolysis kinetics. This sophisticated analysis allowed the unraveling of the inherent complexities of how free enzymes interact with substrates constrained on a highly crowded, curved nanosurface, showcasing a powerful, highly generalized strategy for the design of advanced optical biosensors dedicated to high-sensitivity cancer detection, tissue imaging, and therapeutic monitoring.

4. Fundamental Characterization and Theory

A profound takeaway from the symposium was the collective emphasis on the critical need for next-generation tools and advanced theoretical frameworks capable of correlating individual structural heterogeneity with macroscopic ensemble performance. In the past, characterization methods typically relied on bulk measurements that averaged the properties of trillions of

nanoparticles simultaneously. However, understanding the unique features of individual nanocrystals has become paramount. The presentations of this symposium highlighted a concerted push toward tracking chemical transformations at the single-entity level, modeling non-classical electronic behaviors, and mapping the hidden, diffuse boundaries that govern hybrid materials.

4.1 High-Throughput Single-Particle Imaging and In Situ Kinetics

Prof. Sara Skrabalak outlined the critical need for high-throughput tools and methods capable of screening single-nanocrystal properties to address the long-standing challenges of sample heterogeneity. Even within highly optimized, state-of-the-art colloidal batches, individual nanocrystals inherently display a wide distribution of structural features, such as distinct crystal planes, edges, and surface defects. This heterogeneity represents a double-edged sword: while it offers rich opportunities to discover unique structures with useful properties, it simultaneously confounds conventional bulk property measurements—such as standard ensemble absorption spectroscopy or cyclic voltammetry—where critical minority features are frequently masked by the overall average. To solve this characterization bottleneck, Skrabalak presented recent breakthroughs developed by the Center for Single-Entity Nanochemistry and Nanocrystal Design, focusing on Calcite-assisted Localization and Kinetics (CLoCK) microscopy. CLoCK microscopy operates as a powerful high-throughput screening tool that effectively encodes spectral data into optical images. This enables researchers to rapidly extract the precise size and spatial orientation of individual nanocrystals in real time. Furthermore, Skrabalak highlighted the utility of CLoCK microscopy for *in-situ* tracking of metal nanocrystal dissolution and growth dynamics.[22, 23] By integrating this high-throughput optical technique with electrodeposition directly onto nanocrystal seeds, the research groups at the center led by Skrabalak can visualize the exact origins and propagation features of nanocrystal growth as it unfolds. This approach bridges the gap between single-particle tracking and statistical ensemble analysis.

4.2 Quantum Chemical Modeling vs. Classical Electrodynamics

Shifting the focus from experimental imaging to fundamental physical theory, **Prof. George Schatz** highlighted the necessity of employing quantum-chemistry methods rather than classical electrodynamics to describe high-performance plasmonic phenomena. Plasmons are collective excitations of electrons where the excited state involves a complex superposition of electron-hole

pairs. Traditionally, the optical behavior of these materials has been modeled using classical electrodynamics coupled with empirical dielectric functions. However, Schatz noted that classical models fail to describe specific spectroscopic properties or pathways involving explicit charge transfer between a metal surface and adsorbed molecules.[24] These quantum-mechanical pathways are central to driving surface-enhanced Raman scattering (SERS) and plasmon-induced photocatalysis. His group utilizes advanced quantum chemistry codes applied to small metal clusters to accurately model metal/adsorbate systems. They discovered that calculations performed on clusters just a few nanometers in size serve as excellent, scalable models for the precise chemical effects in SERS and photocatalysis typically observed in much larger particles spanning the 10 to 100 nm range. Because standard electronic structure codes become computationally prohibitive as atom counts scale up, Schatz detailed their recent development of new theoretical frameworks utilizing the Density Functional Based Tight Binding (DFTB) semiempirical method. This specialized tight-binding approach enables accurate simulation of the quantum electronic environments of complex nanoparticles containing up to 1,000 atoms, providing a predictive roadmap that directly links atomic cluster physics to macroscopic plasmonic performance.

4.3 Surface Complexes and Visible-Light Oxide Photocatalysis

Providing an elegant solution to the limitations of wide-bandgap semiconductor photocatalysis, **Prof. Yugang Sun** demonstrated how surface chemistry can be exploited to drive visible-light reactions without relying on expensive noble metals. Desulfurization is a vital process in chemical synthesis, essential for producing new target molecules and accessing highly reactive carbon radicals. However, driving these reactions photocatalytically under broadband visible light illumination has traditionally required expensive noble metal complexes and strictly controlled, inert atmospheres. Sun's group bypassed these requirements by utilizing inexpensive titanium oxide (TiO_2) nanoparticles as active photocatalysts to facilitate desulfurization and subsequent C-C coupling reactions with alkenes under ambient conditions.[25] Because pristine TiO_2 nanoparticles do not naturally absorb visible light, Sun's strategy relies on the adsorption of reactant thiol species directly onto the nanoparticle surface. This localized adsorption triggers the formation of distinct, colorful surface complexes that effectively shift the material's light-absorption profile into the visible spectrum. Upon visible light absorption, these surface complexes facilitate efficient charge migration across the interface, generating the critical reactive intermediates necessary to drive

desulfurization under air. This presentation demonstrates how even simple surface-adsorbate interactions can fundamentally alter the electronic and optical properties of traditional "white oxide" nanomaterials.

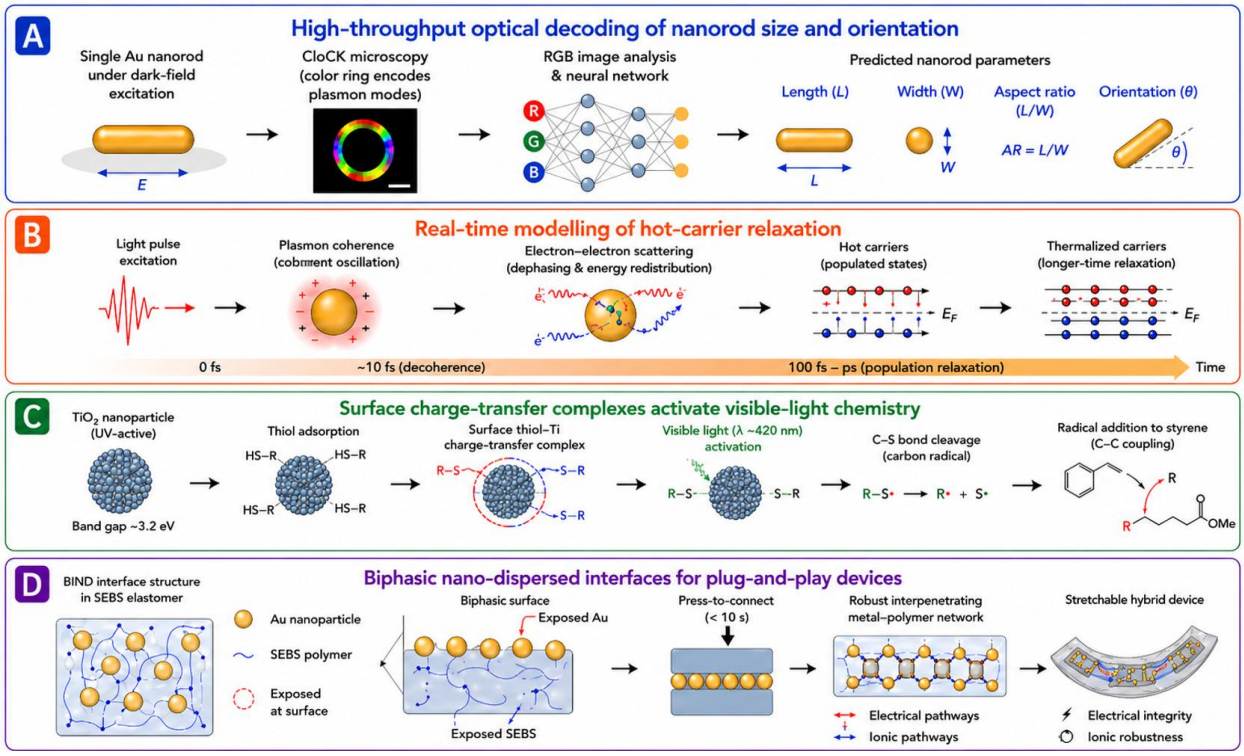

Figure 4. Advanced characterization, theory, and interfacial engineering reveal hidden structure-function relationships in nanomaterials. (A) High-throughput all-optical decoding of gold nanorod size, aspect ratio, and orientation using engineered scattering images.[23] (B) Real-time theoretical modeling of plasmon dephasing, electron–electron scattering, and hot-carrier relaxation in metallic nanostructures.[24] (C) Surface charge-transfer complexes on TiO_2 nanoparticles enabling visible-light-driven desulfurization and C–C coupling chemistry.[25] (D) Biphasic metal–polymer nano-dispersed interfaces providing robust electrical and mechanical connections in stretchable hybrid devices.[26]

4.4 Mapping Diffuse Nanoparticle-Polymer Interfaces

Concluding the session with an exploration of soft-hard hybrid material boundaries, **Prof. Xiaodong Chen** reevaluated the nature of metal-polymer interfaces. These interfaces play a decisive role in dictating the performance, conductivity, and structural stability of flexible electronics, wearable sensors, functional coatings, and advanced energy devices.[26] While researchers routinely visualize this interface as a sharp, well-defined boundary—with pristine

metal resting on one side and bulk polymer on the other—Chen's recent work reveals a completely different morphological reality. When metals meet polymers, tiny metal nanoparticles can spontaneously diffuse into the underlying polymer matrix, creating a hidden, transitional zone that can extend tens to hundreds of nanometers beneath the apparent surface. Chen shared the story behind discovering this diffusion-driven zone, illustrating that this embedded boundary layer is crucial for governing how the two dissimilar materials bond, how they conduct electricity and heat, and how stable they remain over long-term operation. By actively managing and manipulating this nanoparticle diffusion process rather than treating it as an uncontrolled defect, Chen's group demonstrated that they can precisely tune the mechanical strength, electrical performance, and bioelectronic sensing capabilities of next-generation flexible devices, turning a hidden structural challenge into a versatile engineering asset.

5. Future Horizons: Opportunities and Challenges in Nanochemistry

The symposium concluded by reinforcing that the field of nanochemistry has successfully transitioned from a qualitative, "empirical art" into a highly predictive, automated science. As highlighted by Prof. George Schatz, the integration of quantum chemistry with semiempirical methods now enables rigorous descriptions of the electronic structure of nanoparticles comprising up to 1,000 atoms. As with any profound technological paradigm shift, this digital and theoretical maturity brings a suite of transformative opportunities and formidable challenges, both of which will undoubtedly define the next decade of materials design.

The most exhilarating frontier lies in the realization of truly autonomous, closed-loop nanolabs. By tightly coupling high-throughput DFT calculations and ML engines with automated robotic synthesis, the next generation of materials discovery will largely bypass traditional trial-and-error human intervention. Instead of manually troubleshooting recipes, AI-driven platforms will independently conceptualize, synthesize, and analyze complex nanomaterials in real time—rapidly navigating vast multi-dimensional spaces of compositional, dimensional, and surface properties to isolate optimized catalysts or optical probes. Concurrently, merging programmable biological frameworks (such as DNA origami and protein voxels) with highly anisotropic inorganic nanostructures yields unprecedented control over physical and chemical properties, opening new pathways for "intelligent" therapeutics. Such smart nanomedicines will move beyond passive payload delivery to actively navigate complex cellular networks, utilize high-precision

nanothermometry to sense localized disease states, and dynamically alter their geometric conformations to execute targeted, lock-and-key therapeutic interventions.

Despite this immense promise, several structural roadblocks remain. High-throughput nanomaterials discovery via autonomous synthesis is intrinsically limited to small-scale, tightly regulated laboratory settings. Translating these automated discoveries to industrial production introduces a massive scale-up paradox, where materials must be processed in far more complex, dynamically fluctuating macroscale environments where strict kinetic control is difficult to maintain. Furthermore, fully integrating autonomous synthesis with automated characterization within a self-driving lab presents severe physical and computational bottlenecks. Inline optical methods provide rapid, real-time kinetic tracking but lack spatial and structural refinement, whereas high-resolution imaging and scattering techniques require intensive sample preparation, causing a detrimental informational lag. Seamlessly routing delicate, air-sensitive colloidal streams through microfluidic networks without risking sample contamination or altering the sensitive structural identity of the nanocrystals presents an immense fluidic engineering challenge. Additionally, ML models face severe "data friction" due to the inherent structural heterogeneity of nanomaterials, where ensemble bulk averages frequently mask highly reactive minority facets and localized defects. Overcoming this requires the development of adaptive, goal-oriented software architectures capable of dynamically parsing noisy analytical signals to optimize physical reaction parameters on the fly. Ultimately, without a unified, standardized digital infrastructure for sharing both successful and failed synthetic data, machine learning models will remain limited by fragmented, localized training sets.

Parallel challenges emerge when deploying sophisticated, responsive nanomedicines into complex living organisms, moving them from sterile, well-defined environments into a chaotic and reciprocal biological interface. Successfully executing these advanced nanoarchitectures demands a profound, fundamental mastery of the nano-bio interface. It requires rigorous, multi-scale mapping of long-term tissue distribution, clearance pathways, and real-time ‘in vivo’ degradation to overcome intricate physiological barriers. This task is heavily complicated by the extreme sensitivity of the fluid-nanocrystal boundary, where the spontaneous thermodynamic displacement of engineered surface ligands by surrounding biomolecules can compromise colloidal stability, trigger unintended immune responses, or neutralize the particle's tailored therapeutic and sensing functionalities. Moreover, the dense steric crowding and high local

curvature of these nanosurfaces fundamentally alter standard reaction and delivery kinetics, while the propensity of ultra-small particles to spontaneously diffuse into adjacent matrices creates hidden transitional zones that complicate structural stability and long-term therapeutic performance.

In summary, this inaugural award symposium not only honored two pioneering figures in nanochemistry—Profs. Dong Qin and Luis M. Liz-Marzán—but also charted a vibrant roadmap for a discipline that is rapidly becoming predictive, automated, and biologically integrated. The emerging opportunities are vast and bounded primarily by our collective imagination; however, their ultimate realization hinges upon our ability to precisely map, model, and manage these hidden, diffuse boundaries.

Author Information

Author Contributions

The manuscript was written through the contributions of all authors. All authors have given approval to the final version of the manuscript.

Notes

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