COMMENT

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Supramolecular materials in life sciences: Recent advances and future directions

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The convergence of materials science and biotechnology has catalyzed the development of innovative platforms, including nanotechnology, smart sensors, and supramolecular materials, significantly advancing the progress in the field of life sciences [1–7]. Among them, supramolecular materials have garnered increasing attention in life sciences owing to their distinctive self-assembly capabilities and intelligent responsiveness [8–12]. Supramolecular materials can self-assemble simple molecular units into polymer structures with specific functions through non-covalent interactions (hydrogen bonding, π–π stacking, hydrophobic interactions, electrostatic interactions, etc.) to form micelles, vesicles, nanofibers, and three-dimensional networks [13–22]. The self-assembly of supramolecular materials exhibits a high degree of controllability and can dynamically modulate their structure and function in response to external stimuli, including temperature, pH, light, or chemical agents [23–26]. This adaptability presents an innovative approach to development in life sciences [27–30].

At present, supramolecular therapeutics have been widely used in the field of life sciences. For example, supramolecular drug carriers have been demonstrated to significantly enhance drug loading capacity [31–33]. In addition, these carriers have multiple stimuli-response capabilities, which can achieve precisely controlled drug release in response to acid, light, or redox changes in abnormal microenvironments such as tumors [34–36]. This property of supramolecular materials significantly reduces the problems of low drug solubility, uneven distribution, and side effects that exist in traditional delivery systems [37–40]. Mao, Yu and co-workers developed a novel mRNA cancer vaccine using supramolecular lipid nanoparticles as a delivery platform to co-deliver tumor antigen-encoding mRNA and TLR7/8 agonist (R848) to dendritic cells (DCs) for enhanced antitumor effects (Figure 1a) [41]. Among them, *β*-cyclodextrin (*β*-CD)-modified ionizable lipids (Lip-CD) incorporated R848 into mRNA vaccine species through noncovalent host–guest complexation, promoting DC maturation and antigen presentation after vaccination, and greatly improving the stability and bioavailability of R848 in biomedical applications. Furthermore, Chen and co-workers reported that a supramolecular albumin nanoparticle modified based on azocalix[4]arene was capable of simultaneously delivering hydroxychloroquine (HCQ) and mitochondrial-targeting Type I photosensitizer (SMNB) for hypoxic tumor therapy (Figure 1b) [42]. The synergistic effects of HCQ-mediated mitophagy inhibition and SMNB-induced reactive oxygen species overproduction disrupted mitochondrial autophagic flux. This dual action amplified oxidative stress and autophagic dysfunction, ultimately inducing tumor cell apoptosis.

In addition, with the development of the concept of diagnosis and treatment integration, the design of supramolecular imaging probes is becoming increasingly multifunctional, which can be combined with therapeutic drugs to form a "diagnosis and treatment integration" platform. For example, by introducing fluorescence or magnetic resonance imaging functional groups into supramolecular self-assembled systems, probes with excellent biocompatibility and targeting can be constructed [43–45]. These probes can generate pronounced signals in specific pathological regions *in vivo*, thereby achieving high-resolution imaging [46]. This platform not only enables precise early diagnosis of diseases but also effectively treats lesions through mechanisms such as targeted drug release or photothermal and photodynamic therapies, thereby providing more possibilities for precision medicine and personalized therapy [47–49]. For example, Zhou, Wang, Mao and co-workers designed a theranostic metallacycle using perylene bisimide fluorophore and tetraphenylethylene-based di-Pt(II) organometallic precursor as building blocks (Figure 1c) [50]. Through fluorescence resonance energy transfer, perylene bisimide fluorophore shifted the characteristic optical signals to the near-infrared region. Then the metallacycle molecule was self-assembled with GSH-responsive macromolecule to form nanoparticles. These nanoparticles can target tumor cells and tissues, enabling near-infrared imaging-guided *in vivo* radiotherapy. In addition, Zhang, Lin and co-workers constructed supramolecular fluorescent probes by combining cyanine dyes with a *β*-CD polymer using a multivalent molecular self-assembly technique (Figure 1d) [51]. The stability of supramolecular probes was effectively improved by the multivalent host–guest interaction between cyanine dyes and *β*-CD polymer. Furthermore, supramolecular non-covalent interactions enable specific recognition and signal transduction of biomolecules [52, 53]. By exploiting the dynamic reversibility and molecular self-assembly properties of supramolecular materials, highly sensitive and selective detection of targets (e.g. proteins, nucleic acids and small molecule metabolites) can be achieved through host–guest recognition mechanisms. This involves specific binding between the macrocyclic host (such as cyclodextrin, cucurbituril, calixarene or pillararene) and the target molecule [54–60]. Recently, Tian and co-workers developed a supramolecular fluorescent chemosensor by exploiting the host–guest interaction between cucurbit[*n*]uril and naphthalimide-derived dye, with acridine orange serving as the guest reference for quantitative detection (Figure 1e) [61]. This supramolecular sensor can be used for real-time imaging and quantification of norepinephrine dynamics in mouse brain regions, achieving a temporal resolution of approximately 190 ms. Supramolecular chemistry has also achieved remarkable progress in bioinspired materials and regenerative medicine [62]. Sun, Fu, Dong, Liu and co-workers developed a novel DNA-based supramolecular hydrogel system for regeneration-directed artificial skin, with a multilayered architecture designed to mimic the natural skin matrix [63]. Li and co-workers constructed a hyaluronic acid/β-cyclodextrin supramolecular assembly for sustained delivery of insulin-like growth factor-1 and demonstrated controlled release kinetics of bioactive insulin-like growth factor-1 [64].

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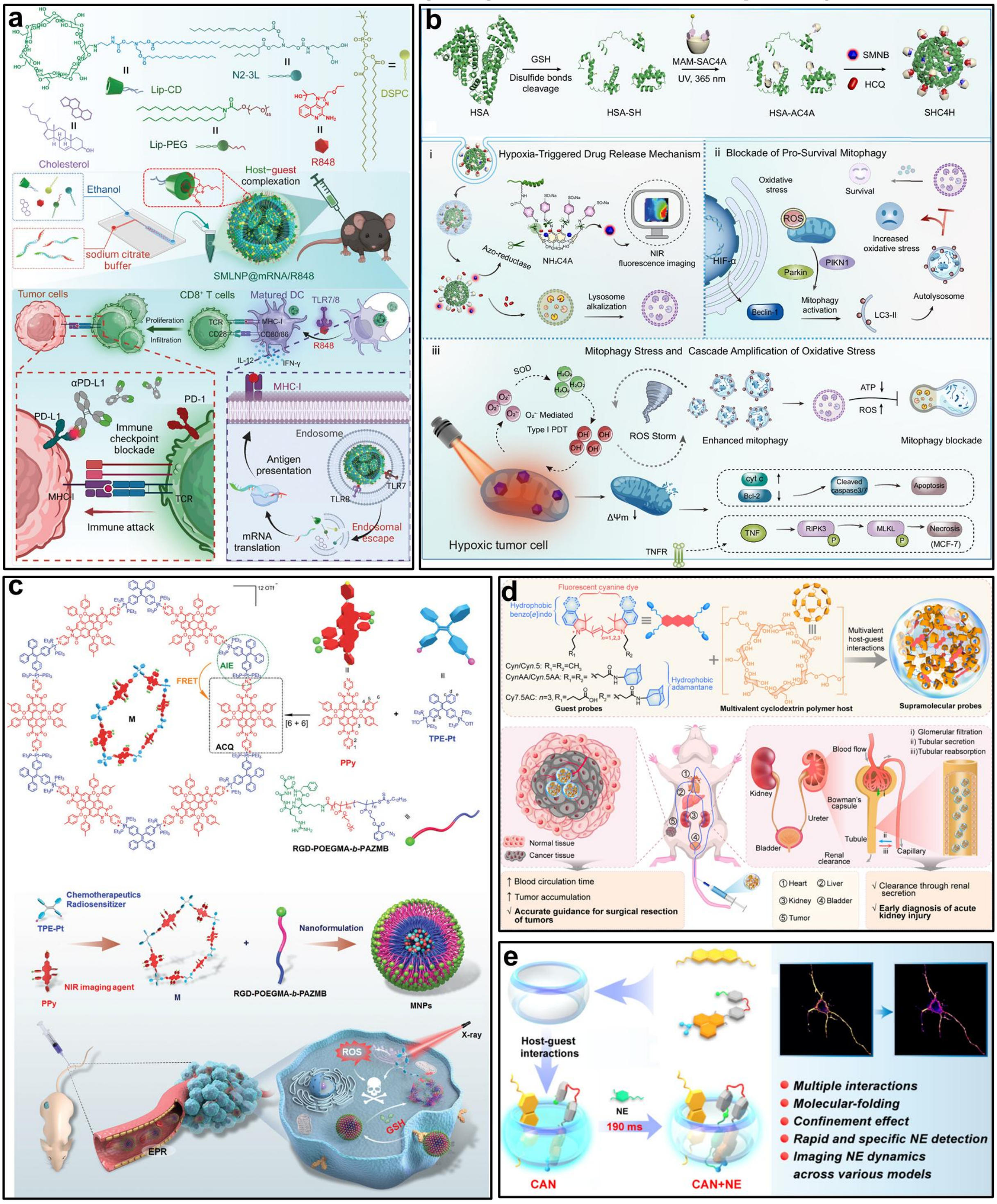

Figure 1 Applications of supramolecular materials in drug delivery (a, b), bioimaging (c, d), and supramolecular biosensors (e). Reproduced with permission. Qi S, Zhang X, Yu X, et. al. Supramolecular Lipid Nanoparticles Based on Host–Guest Recognition: A New Generation Delivery System of mRNA Vaccines for Cancer Immunotherapy. *Adv Mater* 2024;36(23):2311574. Copyright 2024, WILEY. Reproduced with permission. Wang W, Yao SY, Luo J, et. al. Engineered Hypoxia-Responsive Albumin Nanoparticles Mediating Mitophagy Regulation for Cancer Therapy. *Nat Commun* 2025;16(1):596. Copyright 2025, Springer Nature. Reproduced with permission. Ding Y, Tong Z, Jin L, et. al. An NIR Discrete Metallacycle Constructed from Perylene Bisimide and Tetraphenylethylene Fluorophores for Imaging-Guided Cancer Radio-Chemotherapy. *Adv Mater* 2022;34(7):e2106388. Copyright 2022, WILEY. Reproduced with permission. Ding Y, Tong Z, Jin L, et. al. An NIR Discrete Metallacycle Constructed from Perylene Bisimide and Tetraphenylethylene Fluorophores for Imaging-Guided Cancer Radio-Chemotherapy. *Adv Mater* 2022;34(7):e2106388. Copyright 2022, The American Association for the Advancement of Science. Reproduced with permission. Zhao Y, Mei Y, Sun J, Tian Y, A Supramolecular Fluorescent Chemosensor Enabling Specific and Rapid Quantification of Norepinephrine Dynamics. *J Am Chem Soc* 2025,147(6):5025–5034. Copyright 2025, American Chemical society.

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Due to its dynamic, reversible and adaptive nature, supramolecular chemistry is widely used in life sciences for the development of new biological materials, drug delivery, disease diagnosis and treatment, bionic materials, etc. The following is its core application direction and typical cases (Table 1).

Despite significant advances in supramolecular materials for life sciences, several challenges remain for their practical application (Figure 2).

(1) Supramolecular systems rely on weak interactions, making them vulnerable to interference from factors such as plasma proteins, ionic strength, and enzymes, which may lead to dissociation or non-specific binding. Thus, enhancing their stability in physiological environments is an important area of future research.

(2) Although most supramolecular materials exhibit good biocompatibility, their long-term toxicity, *in vivo* degradation, and clearance mechanisms require further systematic assessment to ensure clinical safety.

(3) Integrating multiple functionalities, such as drug delivery, imaging and sensing into a single platform to achieve multifunctional synergy remains a major challenge that requires further innovation in molecular design and assembly regulation.

Table 1 Applications of supramolecular materials in the field of life sciences

Applications	References
Cancer diagnosis	[3, 5, 9, 13, 20]
Drug delivery	[15, 19, 24, 32, 34, 37, 41–44, 50, 57, 58, 60, 61]
Bioimaging and treatment	[18, 28, 45–47, 49, 59]
Biosensing and detection	[48, 51–56]
Bionic materials	[7, 16, 62–64]

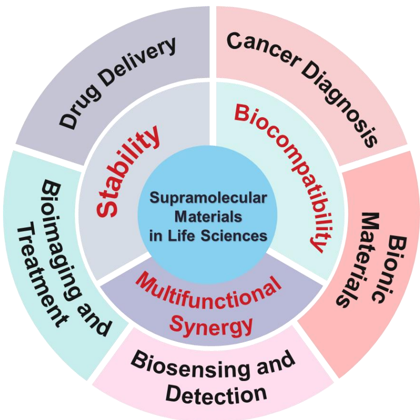

Figure 2 Challenges of supramolecular materials in life sciences

In summary, supramolecular materials have promising applications in life sciences due to their unique self-assembly and smart response properties. By improving the stability and biosafety of materials *in vivo* and realizing multifunctional synergistic effects, supramolecular materials are expected to play a greater role in areas such as precision medicine and intelligent diagnosis in the future. Meanwhile, interdisciplinary collaboration will promote the deep integration of supramolecular chemistry, materials science, and biomedicine, accelerating their transformation from basic research to clinical practice.

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Author Contributions

Zhang WJ: Writing-original draft, Funding acquisition. Zhou J: Review and editing. Zhang WJ and Zhou J: Conceptualization. Zhou J: Supervision.

Competing interests

The authors declare no conflicts of interest.

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