

PERSPECTIVES

DNA-mediated carbon nanotube sorting: progress, mechanisms, and perspectives

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1 Introduction

Single-walled carbon nanotubes (SWCNTs) have remained at the vanguard of materials science since their discovery, functioning as a prototypical quasi-one-dimensional system with exceptional physicochemical, optical, and electronic properties [1]. These properties are intrinsically linked to chiral indices (n, m), which determine the wrapping angle and diameter of the hexagonal carbon lattice (Figure 1a). This structural specificity defines their electronic identity: SWCNTs exhibit metallic behavior when $n - m = 3k$ (where k is an integer), whereas all other configurations function as semiconductors. Despite this potential, as-synthesized SWCNTs typically manifest as stochastic ensembles with a polydisperse distribution of chiralities. Consequently, developing robust, scalable strategies for isolating single- (n, m) SWCNTs has become a pivotal frontier in carbon nanoscience. Traditional sorting methods—including density-gradient ultracentrifugation [2], gel chromatography [3], surfactant-assisted separation [4], and polymer extraction [5]—predominantly rely on non-specific molecular interactions. In contrast, since the seminal work by Zheng *et al.* [6] in 2003, single-stranded DNA (ssDNA) has driven a paradigm shift from simple colloidal dispersions to structure-defined bio-nano hybrids. Leveraging absolute sequence programmability, the ssDNA platform provides unparalleled sequence-specific recognition, enantiomer discrimination, and ordered corona architectures [7]. This approach not only enables the high-purity enrichment of discrete (n, m) species but also inherently bridges pristine SWCNTs to functional bio-nano interfaces. Here, we trace the evolution of DNA-mediated SWCNT isolation and provide our perspectives on this evolving field.

2 DNA-mediated SWCNT recognition and separation

Zheng and colleagues [6] demonstrated that ssDNA can effectively disperse and stabilize individual SWCNTs in aqueous media, forming DNA-SWCNT hybrids anchored by intensive π - π stacking between the aromatic nucleobases and graphitic sidewalls. While the bases serve as hydrophobic anchors, the hydrophilic sugar-phosphate backbone remains exposed, providing colloidal solubility and a high density of negative surface charge (Figure 1b). Subsequent fractionation of these hybrids via ion-exchange

chromatography (IEX) revealed distinct spectroscopic profiles. Typically, early elution fractions are enriched with metallic SWCNTs, while later fractions predominantly contain semiconducting species (Figure 1c, d). This selective elution is dictated by the differential effective surface charge of the hybrids. The high polarizability of metallic nanotubes induces image charges that screen the negative charge of the adsorbed DNA backbone. This localized charge attenuation reduces electrostatic affinity for the anion-exchange resin, facilitating the prioritized elution of metallic nanotubes.

Beyond general dispersion, a sequence-dependent DNA-mediated assembly strategy was subsequently proposed for SWCNT sorting. Through systematic library screening, Zheng *et al.* [8] identified $(GT)_n$ motifs that spontaneously organize into hypothesized helical conformations, stabilized by an intricate network of inter- and intra-strand hydrogen bonds (Figure 1e). This structural regularity renders the hybrid surface charge density exquisitely sensitive to both nanotube diameter and electronic character. The resulting elution profile follows a predictable progression, typically prioritizing smaller-diameter metallic species before transitioning toward larger-diameter semiconducting nanotubes. Notably, the $(GT)_{10}$ sequence was found to effectively decouple metallic from semiconducting nanotubes (Figure 1f) [9], an essential step for fabricating advanced nanoelectronic devices.

Compared with electronic-type fractionation, isolating specific (n, m) chiralities from structurally similar ensembles represents a more rigorous challenge. To address this, Zheng and Semke [10] implemented a tandem strategy, using size-exclusion chromatography (SEC) as a preparatory step to narrow the length distribution prior to IEX. This refinement enhanced resolution for small-diameter species, enabling the high-purity enrichment of (6,4), (9,1), and (6,5) (Figure 1g). The successful fractionation of (9,1) and (6,5) is particularly noteworthy, as these two species possess identical diameters yet exhibit distinct elution behaviors. Such a result provides unequivocal evidence that the separation mechanism transcends simple diameter-dependent charge screening and is instead governed by chirality-dependent molecular recognition, likely rooted in subtle variations of the DNA-wrapping conformation.

Although DNA-SWCNT interactions are dictated by sequence-

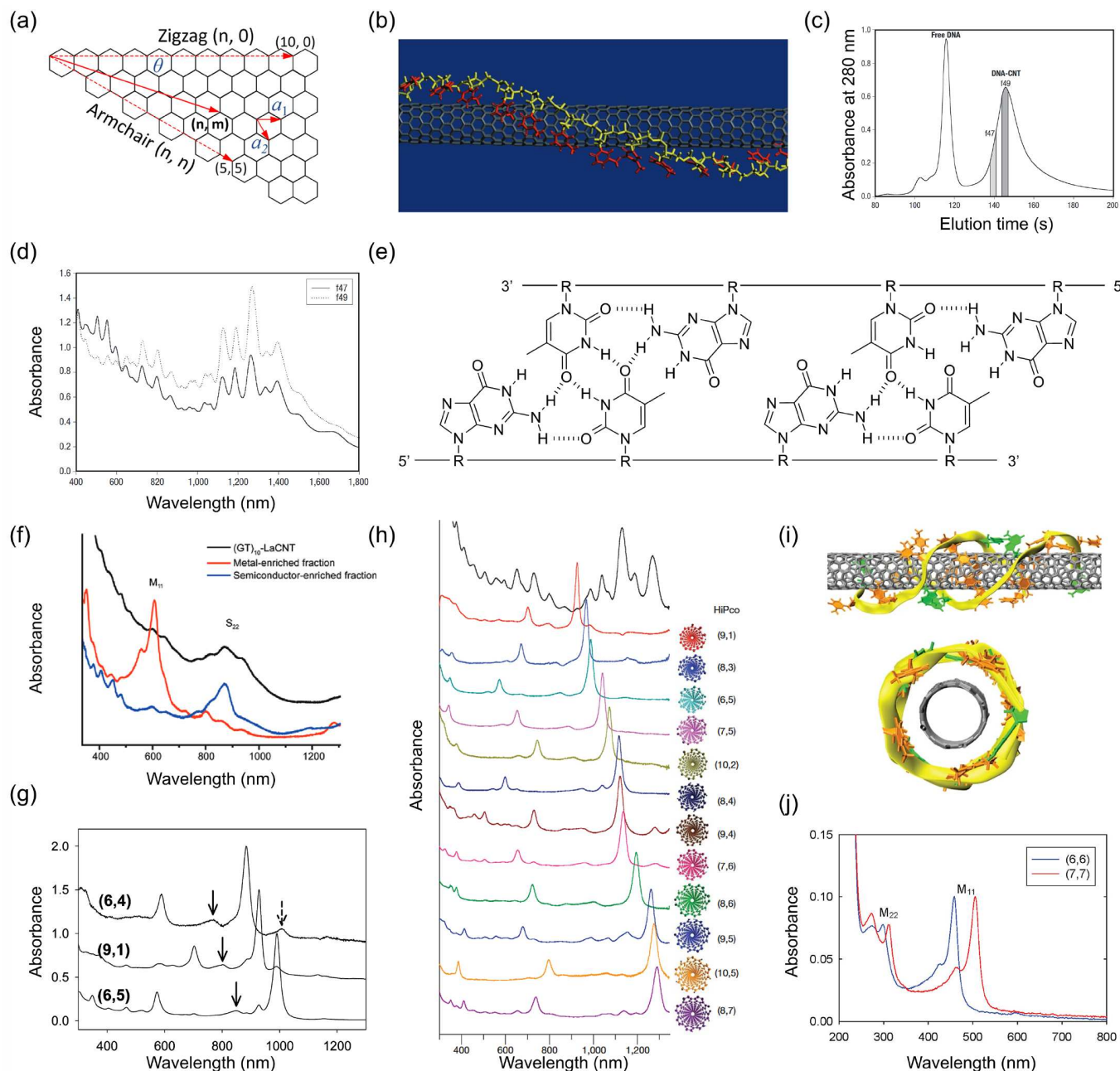


Figure 1 (Color online) Evolution of DNA-mediated SWCNT recognition and separation. (a) Structural schematic of (n,m) chiral indices defining the SWCNT lattice. (b) Binding model of poly(T) wrapped on a $(10,0)$ nanotube, where the nucleobases (red) facilitate π - π stacking with the sidewalls while the phosphodiester backbone (yellow) provides aqueous solubility and interfacial charge. (c) Chromatogram of anion-exchange column separation of DNA-SWCNTs. (d) Absorption spectra of early and later fractions. Reproduced with permission from Ref. [6]. Copyright 2003, Springer Nature. (e) Proposed hydrogen-bonding interactions of DNA strands. (f) Absorption spectra of collected fractions that contain metal- and semiconductor-enriched SWCNTs, respectively. Reproduced with permission from Ref. [9]. Copyright 2008, the Author(s). (g) Absorption spectra of three single-chirality-enriched SWCNT species. Reproduced with permission from Ref. [10]. Copyright 2007, American Chemical Society. (h) Absorption spectra of 12 purified semiconducting SWCNTs. (i) Molecular dynamics model of the resolving sequence $(ATTT)_3$ wrapped on an $(8,4)$ nanotube. Reproduced with permission from Ref. [11]. Copyright 2009, Springer Nature. (j) Absorption spectra of two metallic armchair SWCNTs. Reproduced with permission from Ref. [12]. Copyright 2011, American Chemical Society.

structure synergies, identifying specific resolving sequences within the vast DNA library—approximately 4^{100} candidates available from synthetic oligonucleotides—appeared insurmountable. Tu *et al.* [11] addressed this complexity by establishing a systematic search strategy based on sequence motifs. By strategically developing a sequence pattern expansion scheme to explore the library in a controlled and incremental fashion, they identified more than 20 sequences exhibiting structure-specific recognition for 12 semiconducting SWCNT species (Figure 1h), marking a landmark achievement in chirality sorting. They postulated that the recognition mechanism involves the formation of stable, ordered three-

dimensional DNA barrels around specific nanotubes (Figure 1i). Mechanistically, the effective surface charge density governing elution relies on a cooperative combination of both intrinsic nanotube properties and extrinsic DNA conformations. While polarizability differences dominate electronic-type charge screening, high-resolution chirality sorting is driven by the precise spatial conformation of the DNA wrapping. These sequence-defined wrappings translate the intrinsic electronic identity and curvature of the nanotubes into a unique, macroscopically resolvable surface charge density, which modulates the equilibrium of electrostatic and electrodynamic interactions.

Expanding the scope beyond semiconducting species, the same research group extended this methodology to the isolation of single-chirality metallic species through an evolutionary DNA screening strategy. By employing single-point scanning mutations and motif variations, they successfully purified (6,6) and (7,7) armchair nanotubes (Figure 1j) [12]. This demonstrated the exquisite sensitivity of DNA recognition to both electronic character and lattice structure.

Despite these landmark achievements in chirality isolation, the persistent reliance on IEX-centric separation techniques presents several bottlenecks. The process is inherently time-consuming and often hindered by low recovery rates due to irreversible adsorption on the column resin. These limitations, combined with the requirement for sophisticated instrumentation, impede the scalable separation of single- (n,m) SWCNTs. Consequently, the development of facile, high-efficiency separation protocols suitable for ambient aqueous environments has emerged as a critical imperative for the field.

3 Aqueous two-phase system for the separation of single-chirality SWCNTs

To address the operational constraints of traditional chromatography, aqueous two-phase (ATP) system extraction has emerged as a versatile and efficient alternative. These systems leverage the spontaneous phase separation of polymers to create two distinct, immiscible aqueous environments. Within this biphasic milieu, the selective separation of DNA-SWCNTs is governed by equilibrium partitioning; variations in the solvation energies of specific (n,m) species drive their preferential migration into disparate phases (Figure 2a). Over the past decade, this thermodynamically driven sorting paradigm has significantly expanded the toolkit for DNA-mediated isolation, offering a robust and scalable platform for bulk chirality purification.

In 2014, Ao *et al.* [13] demonstrated the capacity of ATP systems for separating DNA-SWCNTs. These hybrids exhibit asymmetric partitioning between the aqueous phases, which can be precisely tuned by poly(vinylpyrrolidone) (PVP) as a partition modulator. Sequential PVP addition facilitates multiple repartitioning stages, enabling systematic isolation based on unique solvation energy landscapes (Figure 2b). Utilizing a poly(ethylene glycol)/polyacrylamide (PEG/PAM) ATP system, they mapped the partitioning behavior of various DNA-SWCNT complexes (Figure 2c) and successfully purified 15 distinct (n,m) species. Notably, the purification yield of this method is approximately three to four times higher than that of conventional IEX, establishing ATP as a highly efficient methodology for single- (n,m) SWCNT isolation.

Beyond the (n,m) indices, the crystallographic identity of a nanotube is further defined by its enantiomeric handedness, as most species exist as left- and right-handed pairs. Because these enantiomers possess near-identical physical and chemical attributes, their discrimination is significantly more challenging than standard chirality sorting. To overcome this, Ao *et al.* [14] screened DNA libraries composed of binary nucleotides within an ATP system, successfully isolating 23 distinct single- (n,m) SWCNTs (Figure 2d). These isolated species encompass a broad spectrum of electronic structures—including metallic, quasi-metallic, and semiconducting nanotubes—with their specific handedness confirmed via circular dichroism (CD) spectroscopy (Figure 2e). A pivotal discovery was that a single DNA sequence can adopt distinct wrapping conformations on two enantiomers of the same (n,m) species, such as (6,5). This enabled the sequential isolation of both (+) and (−) enantiomers, exhibiting mirror-image CD signals (Figure 2f). These results reveal that DNA-mediated recognition is

sensitive to lattice structure, translating subtle structural differences into divergent solvation energies. Furthermore, these sequence-dependent DNA structural variations resulted in marked differences in photoluminescence behavior and chemical reactivity [14].

Despite the effectiveness of ATP protocols, the extensively used PEG/PAM system is often hindered by interfacial trapping, a phenomenon driven by substantial hydrophilic disparities between two phases. This challenge, coupled with the commercial discontinuation of PAM, pushed researchers to pursue a thermodynamically milder PEG/dextran (PEG/DX) system [15]. This alternative platform effectively circumvents interfacial trapping, enabling high-resolution, iterative separation through sequential PVP addition. Beyond practical advantages, this system provides profound insights into the thermodynamic basis of DNA-mediated recognition. Fundamentally, DNA adopts sequence-specific conformations that dictate unique solvation energies for distinct (n,m) species. While most sequences yield overlapping energetic distributions, a resolving sequence organizes into an ordered structure that narrows the solvation energy distribution for a target (n,m) species. This structural regularity maximizes the energetic differentiation from the mixtures, allowing the ATP systems to probe these thermodynamic signatures and partition single- (n,m) SWCNTs into specific phases (Figure 2g).

Scalability is a paramount advantage of the ATP methodology. In 2025, Lyu *et al.* [16] introduced a series of low-viscosity, cost-effective PEG/salt systems (Figure 2h). This platform maintained high-purity enrichment of (−)(6,5) during a 200-fold scale-up to volumes of 40 mL (Figure 2i), underscoring the potential for macroscopic single- (n,m) SWCNT production. However, these salt-driven systems are frequently hampered by interfacial trapping, which can compromise the resolving capabilities of DNA sequences that were originally validated in polymer/polymer ATP systems.

Notwithstanding the technical viability of ATP systems for isolating single- (n,m) SWCNTs, identifying resolving sequences remains a stochastic and labor-intensive endeavor. The field's continued reliance on heuristic trial-and-error—often yielding low success rates—represents a significant bottleneck for single- (n,m) SWCNT separation. Consequently, establishing systematic, high-throughput screening paradigms is no longer a luxury but a critical imperative for the evolution of the field.

4 Machine learning-guided sequence screening for SWCNT sorting

The rapid evolution of computational science has established machine learning (ML) as a paradigm-shifting framework in materials research. By discerning high-dimensional patterns within experimental datasets, ML algorithms can accurately forecast uncharacterized resolving DNA sequences. Integrating these predictive models into a systematic screening pipeline transitions the field from trial-and-error toward the high-throughput isolation of single- (n,m) SWCNTs.

In 2019, Yang *et al.* [17] demonstrated a predictive framework for resolving sequence discovery by applying ML to a 12-mer CT-rich DNA library. This approach utilized diverse feature engineering techniques—including position-specific and motif-based encoding—to train classification models such as logistic regression (LR), support vector machines (SVM), and artificial neural networks (ANN). Prediction accuracy was refined through an iterative cycle: candidate sequences were experimentally validated via ATP systems, and the resulting data were integrated into the training set to retrain the models (Figure 3a). This recursive optimization elevated the success rate from an initial 10% to over 50%, establishing a data-driven scheme for DNA sequence screening to

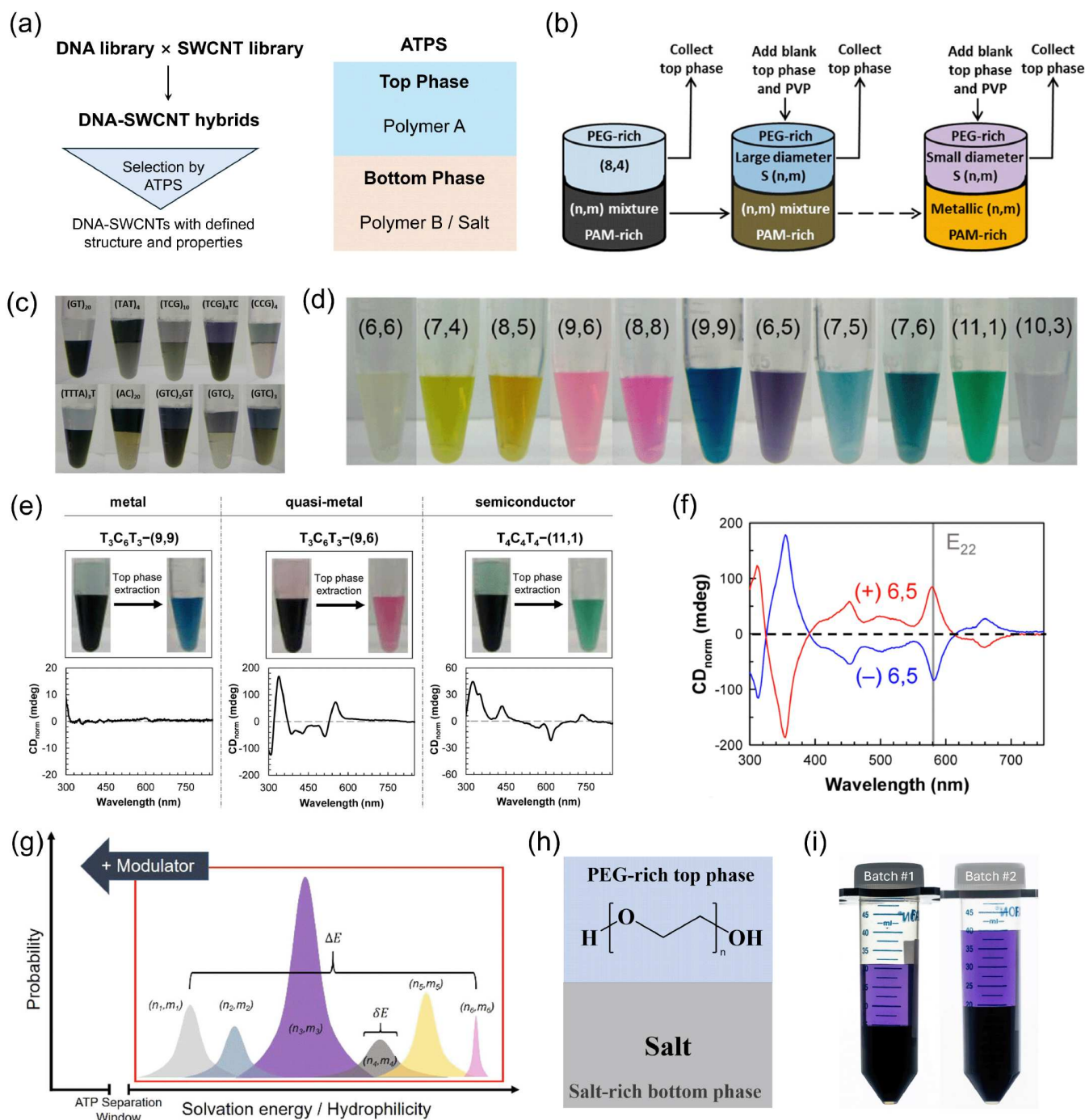


Figure 2 (Color online) ATP systems for SWCNT sorting. (a) ATP selection scheme. (b) Process flow for the sequential addition of PVP, facilitating the multistep extraction of (GT)₂₀-SWCNTs in the PEG/PAM system. (c) Photographs showing the partition of various DNA-SWCNTs in the PEG/PAM system. Reproduced with permission from Ref. [13]. Copyright 2014, American Chemical Society. (d) Photographic library of high-purity, single-chirality SWCNT suspensions isolated via ATP systems. (e) Representative partitioning behavior of three SWCNT species in ATP systems, and their corresponding CD spectra. (f) CD spectra of TTA(TAT)₂ATT-(±)(6,5) enantiomers, demonstrating high-fidelity handedness recognition of DNA. Reproduced with permission from Ref. [14]. Copyright 2016, American Chemical Society. (g) Scheme depicting the solvation energy distribution of various DNA-SWCNT species and the separation window in ATP systems. Reproduced with permission from Ref. [15]. Copyright 2019, American Chemical Society. (h) Schematic of PEG/salt ATP system. (i) Demonstration of large-scale separation of (6,5) via PEG/salt system. Reproduced with permission from Ref. [16]. Copyright 2025, the Author(s).

sort single-(*n,m*) SWCNTs.

In 2022, Lin *et al.* [18] developed an ML-aided systematic search strategy to navigate the vast DNA sequence space for SWCNT sorting. To circumvent the combinatorial explosion of sequence possibilities, they employed a bottom-up approach, initiating the search with short oligonucleotides (e.g., 5-mers) (Figure 3b) and iteratively expanding into a longer sequence library. This hierarchical screening allowed for an exhaustive evaluation of whole sequence landscapes rather than being confined to isolated

combinations. Through a closed-loop cycle of ML-based prediction and experimental validation (Figure 3c), the success rate for identifying effective resolving sequences surged to >90%. This predictive paradigm enabled the high-purity isolation of 22 distinct (*n,m*) species and elucidated that specific G/C motifs function as “super-resolving” patterns for chirality recognition.

To further advance toward specific, targeted chirality sorting, Lin and co-workers [19] recently introduced a deep-learning (DL) enhanced strategy for resolving sequence prediction. By experi-

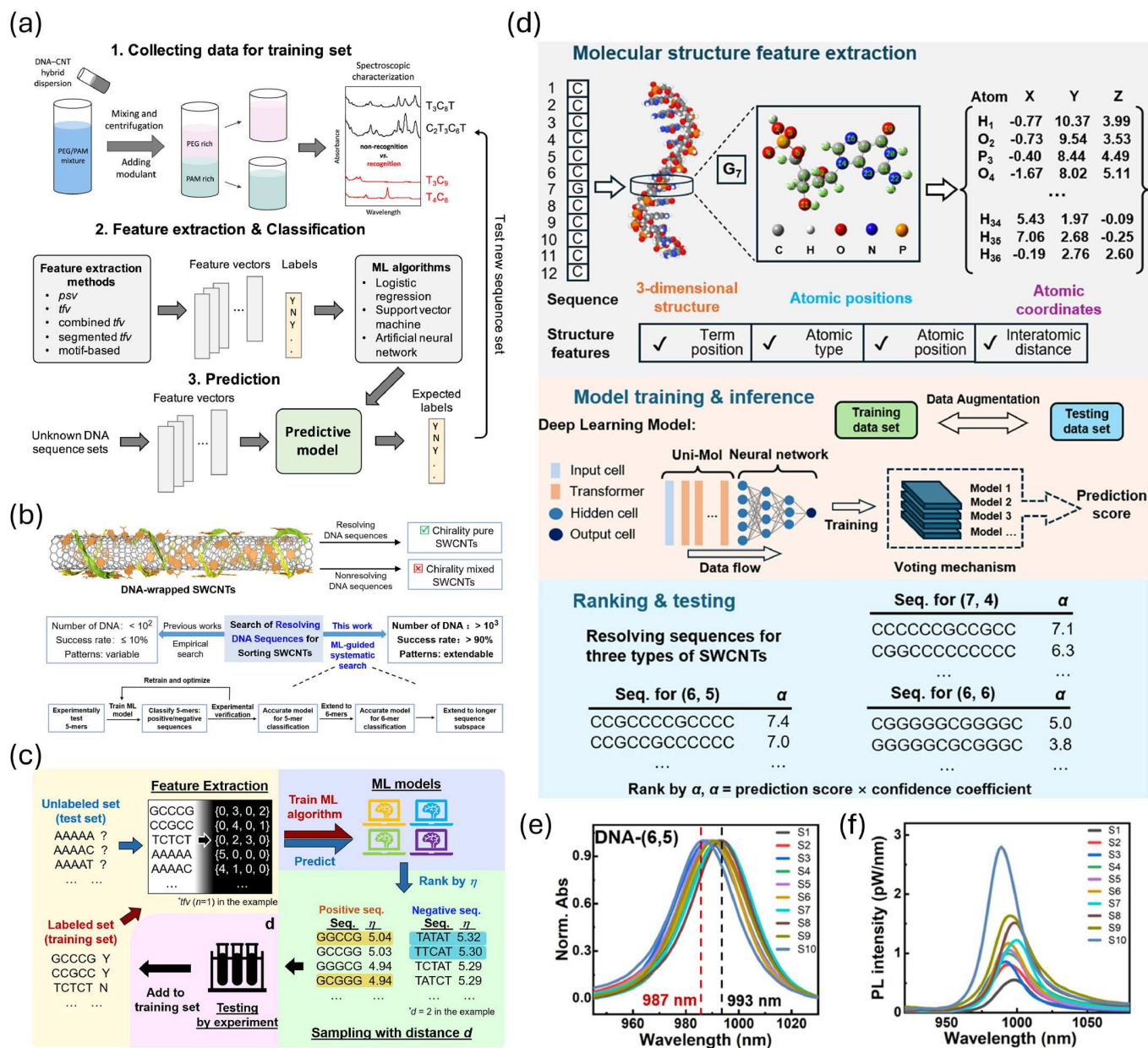


Figure 3 (Color online) ML-guided DNA sequence discovery. (a) Experimental and computational pipeline for the iterative discovery and optimization of resolving sequences. Reproduced with permission from Ref. [17]. Copyright 2019, the Author(s). (b) Schematic illustration of short DNA-wrapped SWCNTs. (c) Workflow of the ML-guided strategy for DNA sequence screening, featuring sequence encoding, consensus prediction across three distinct algorithms, and iterative refinement through ATP-based experimental feedback. Reproduced with permission from Ref. [18]. Copyright 2022, American Chemical Society. (d) Schematic of the DL framework for predicting sequences to sort specific, targeted (n,m) SWCNTs, integrating atomistic-level feature extraction, a voting-enhanced Uni-Mol transformer architecture, and α -score-guided sequence prioritization. (e) Normalized absorption spectra and (f) photoluminescence spectra of ten purified DNA-(6,5), illustrating the sequence-dependent modulation of hybrid optical properties. Reproduced with permission from Ref. [19]. Copyright 2025, American Chemical Society.

mentally screening a library of 216 DNA sequences using ATP systems, they curated a high-fidelity training dataset. Central to this approach is the integration of Uni-Mol into a DL workflow (Figure 3d), which leverages a feature matrix derived from the atomistic-level 3D structural information of DNA molecules. This framework achieved predictive accuracies of 87.5%, 90%, and 70% for (6,5), (6,6), and (7,4) species, respectively. This extensive repertoire enabled a systematic exploration of sequence-dependent optical properties (Figure 3e, f). These findings reveal that distinct resolving sequences adopt unique wrapping conformations even on identical nanotube species—structural nuances that directly dictate the macroscopic functional properties of the resulting bio-nano hybrids.

Despite these gains in screening efficiency, data-driven methodologies impose stringent demands on dataset quality and volume.

Constructing robust models requires a critical mass of validated resolving sequences, yet sourcing these from expansive libraries still entails substantial labor and cost investment, often leading to a suboptimal cost-to-benefit ratio. Crucially, because current models are typically trained within restricted sequence libraries and protocol-specific experimental conditions, their predictions should be explicitly viewed as domain-limited sequence prioritization tools rather than universal predictors of DNA-SWCNT recognition. Furthermore, current validation protocols are frequently biased toward the highest-scoring predictions, leaving the model's fidelity across the broader sequence landscape largely unexamined. Most critically, the latent features extracted by complex algorithms remain difficult to correlate with physical principles, creating a persistent interpretability gap. This reliance on statistical power

obscures the fundamental molecular mechanisms at the DNA-SWCNT interface, which remains the “missing link” for transitioning from empirical prediction toward truly rational, structure-based design.

5 Structural determination and mechanistic insights into DNA-SWCNT interfaces

To bridge the gap between empirical success and mechanistic clarity, recent efforts have shifted toward high-resolution structural characterization. For decades, the field relied on hypothesized interfacial architectures to rationalize how DNA assemblies modulate solvation energies and facilitate selective ATP partitioning. However, the fundamental thermodynamic drivers of ordered assembly and the quantitative structural parameters of these hybrids remained largely elusive. This critical knowledge gap stemmed primarily from the lack of analytical techniques capable of resolving the structures of DNA-SWCNTs.

In the absence of direct high-resolution imaging, computational simulations initially provided the foundational structural blueprints. Roxbury *et al.* [20] utilized replica exchange molecular dynamics (REMD) to demonstrate that multiple DNA strands can self-assemble into thermodynamically stable, ordered wrappings on the nanotube surface (Figure 4a). Their findings revealed that molecular recognition is governed by a dual-synergy mechanism: the sequence-specific ability to form an intra-strand self-stitching network and a precise geometric match between the resulting helical conformation and the nanotube diameter.

Definitive experimental validation of these interfacial structures was recently achieved through the first sub-nanometer resolution characterization of DNA-SWCNT hybrids by Lin *et al.* [21]. Leveraging high-resolution atomic force microscopy (AFM), they determined the structures of five distinct hybrids (Figure 4b). These findings revealed that the resolving sequence TTA(TAT)₂ATT organizes into a highly ordered, left-handed helical wrapping on (–)(6,5). This specific conformation is characterized by a helical pitch of 1.68 nm and a hybrid diameter of 1.91 nm. These parameters were further corroborated by orthogonal cryo-electron microscopy (cryo-EM) reconstructions (Figure 4c). In stark contrast, the non-resolving sequence (T₃C₃)₂C₃ forms a stochastic, disordered coating on the identical (–)(6,5) (Figure 4d), providing direct evidence that ordered assembly is a structural hallmark of successful chirality recognition. Further structural analysis of TTA(TAT)₂ATT on the (+)(6,5) enantiomer elucidated different structural parameters, demonstrating the remarkable conformational plasticity of DNA in response to the nanotube chirality and handedness. The analyses of C₃(CCG)₃(+)(9,1) and G₂C₈GC(–)(10,0) hybrids (Figure 4e, f) demonstrated that interfacial configurations are not merely incidental but meticulously governed by the interplay between DNA sequence and nanotube chirality, providing a physical basis for chiral-selective recognition.

These precise structural parameters offer molecular insights into the underlying separation mechanisms. Structural analysis elucidates that TTA(TAT)₂ATT wraps around (–)(6,5) with a periodicity of nine bases per helical turn, facilitating a cooperative hydrogen-bonding network (HBN). Within this network, all adenine (A) bases are stabilized through intermolecular or intramolecular pairing with thymine (T) (Figure 4g). This cumulative bonding energy fundamentally ensures the stability of the ordered conformation. Sequence mutations that disrupt the HBN eliminate the resolving capability of the sequence, whereas modifications that maintain or reinforce the network preserve the ability to isolate high-purity nanotubes (Figure 4h).

The structural elucidation of DNA-SWCNT hybrids provides a

definitive answer to a question that has spanned over two decades: the existence of ordered interfacial architectures. By establishing the HBN, this research clarifies how precise hydrogen-bonding interactions stabilize these ordered architectures, finally shifting the field toward the more rational design of resolving sequences. Nevertheless, current spatial resolution still falls short of atomic-scale precision. Consequently, the fundamental mechanisms governing the precise registry between the nucleobases and the hexagonal carbon lattice remain largely veiled. Bridging this remaining knowledge gap represents the next frontier—a pursuit essential for unlocking the ultimate potential of DNA-mediated SWCNT sorting and the realization of bespoke bio-nano architectures.

6 Summary and outlook

The field of DNA-mediated SWCNT sorting has reached a pivotal juncture, having successfully expanded the library of (*n,m*) species through the discovery of hundreds of resolving sequences. Yet, a fundamental challenge persists: the discovery process remains largely decoupled from universal design principles, forcing a continued reliance on labor-intensive, empirical screening rather than a predictive forward-design framework. Even with the integration of machine learning, the acquisition of resolving sequences is hindered by a fragmented understanding of the DNA-SWCNT interfacial interaction logic. The recent development of a structure-centric workflow—integrating AFM-based structural determination, HBN modeling, and rational sequence design—marks a shift toward structure-directed engineering. However, the heavy reliance on high-resolution AFM remains a critical bottleneck. Future progress must prioritize “less-instrumentation” strategies that translate high-resolution structural “ground truths” into scalable, high-throughput discovery platforms.

Realizing these methodological advancements requires a fundamental conceptual shift: purified single-(*n,m*) SWCNTs featuring ordered DNA conformations must be conceptualized as precisely defined molecular hybrids rather than simple bipartite mixtures. Analogous to the genetic double helix or protein folding, these ordered wrappings constitute unique secondary structures that endow the bio-nano interface with specific functional identities. Embracing this hybrid framework illuminates a cascading landscape of future opportunities, unfolding naturally from immediate technological realities to far-horizon scientific frontiers.

The most immediate and practical horizon for structure-defined hybrids lies in advanced molecular sensing. Recent studies underscore that within both optical and electrical sensing regimes, purified SWCNTs possessing ordered DNA configurations exhibit enhanced sensitivity and specificity [21–24]. By orchestrating arrays of DNA-SWCNT hybrids with controlled helical pitches and chiralities, researchers can construct high-precision, cross-reactive sensor platforms. Operating analogously to biological olfactory receptors that decipher complex odors through differential response profiles, these arrays execute accurate molecular fingerprinting [25]. This capability establishes a reliable framework for real-world diagnostics in heterogeneous matrices, ranging from the isolation of disease biomarkers in physiological fluids to liquid biopsy-based cancer detection [26]. Fully actualizing this biomimetic platform now necessitates the systematic expansion of the purified DNA-SWCNT library and the exhaustive compilation of these multi-dimensional response signatures.

Stepping beyond sensing, the next evolutionary stage of this field leverages these deterministic architectures to achieve breakthroughs in quantum material fabrication. As structure-directed engineering matures, the ordered nature of these hybrids provides ideal physical templates for site-specific, covalent functionalization.

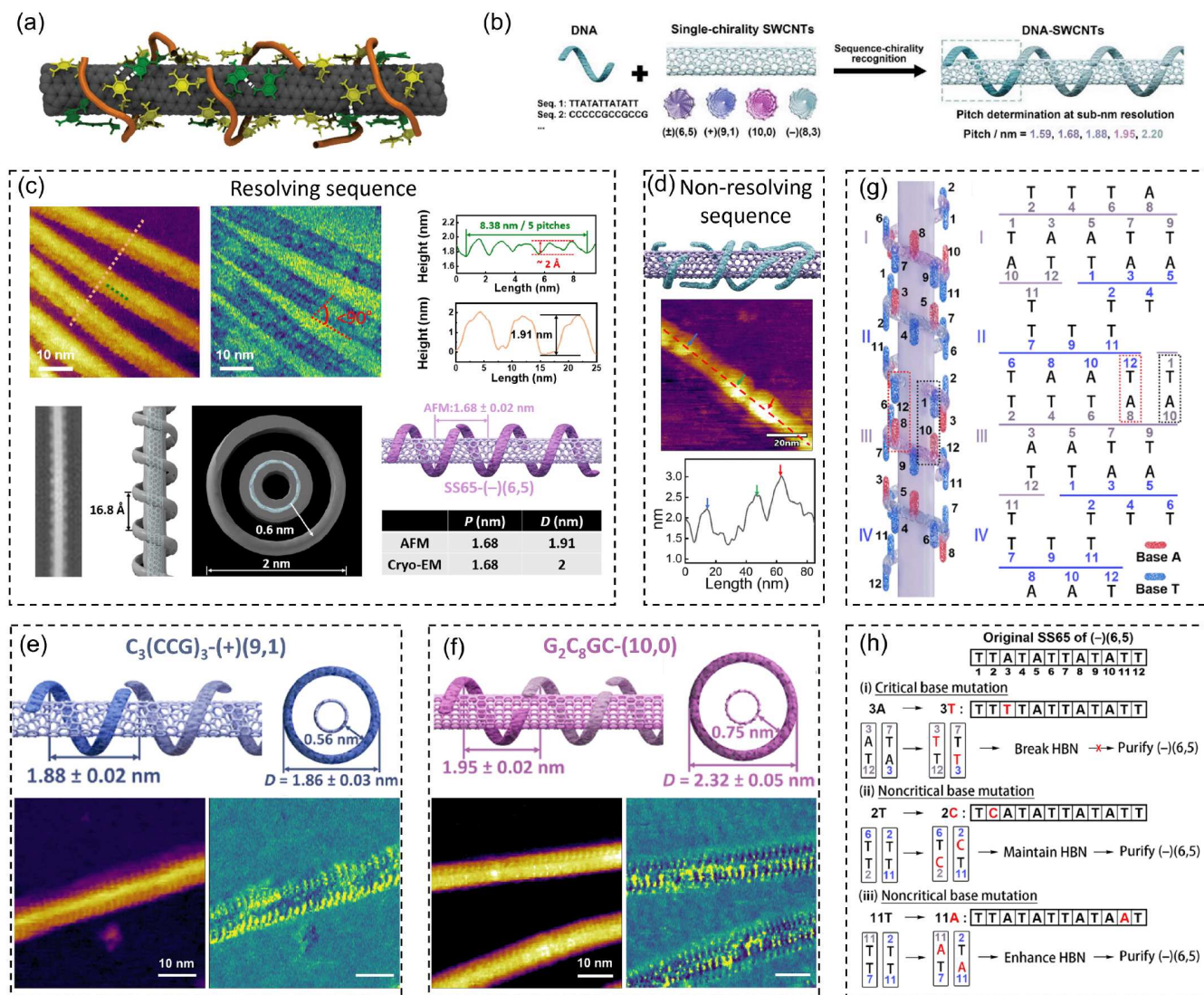


Figure 4 (Color online) High-resolution structural determination and the HBN model. (a) Computational model of (TAT)₄ helically wrapped on a (6,5) SWCNT. Reproduced with permission from Ref. [20]. Copyright 2012, American Chemical Society. (b) Schematic representation of sequence-specific DNA wrapping on single-chirality (n,m) SWCNTs, forming ordered DNA helices with various periodicities. (c) Structural determination of TTA(TAT)₂ATT-(6,5) by AFM and cryo-EM. (d) Structural characterization of the non-resolving sequence (T₃C₃)₂C₃ on -(6,5), revealing a stochastic, disordered coating. (e, f) Schematic and corresponding AFM images of C₃(CCG)₃-(+)(9,1) and G₂C₈GC-(10,0). (g) 3D and 2D HBN models proposed for TTA(TAT)₂ATT-(6,5). (h) Resolving sequence design for -(6,5) by targeted point mutations of the TTA(TAT)₂ATT template. Reproduced with permission from Ref. [21]. Copyright 2025, the Author(s).

By utilizing the sub-nanometer registry and grooved geometry of the ordered DNA corona, chemical modifications can be guided to precise atomic coordinates rather than relying on stochastic chemical attacks [27]. This spatial control is essential for homogeneously introducing defect-induced centers, creating a reliable and scalable pathway toward single-photon-emitting organic quantum materials, and even organic superconductors [28].

In a broader context, a significant frontier emerges at the convergence of lattice physics and complex bio-assemblies. This vision capitalizes on the mechanism of chiral-induced spin selectivity (CISS), wherein the helical geometry of DNA is utilized to intrinsically guide spin-polarized currents [29]. Interfacial coupling between these ordered DNA templates and the intrinsic electronic structures of SWCNTs may establish a structurally defined interface. This synergy holds immense potential to elevate spin-filtering efficiencies, offering a sequence-controlled macromolecular platform for next-generation spintronics.

Ultimately, the continuous expansion of the hybrid library, complemented by increasingly sophisticated functionalization

strategies, will yield complex assemblies that exhibit distinct emergent properties. By integrating the mechanical, electrical, and optical properties of SWCNTs with the inherent biocompatibility and information-storage capacity of DNA, these tailored hybrids transcend the properties of their individual constituents. These advancements will establish a transformative class of hierarchical functional materials, bridging synthetic nanostructures with biological target specificity to address key challenges in next-generation electronics and molecular medicine.

Conflict of interest

The authors declare no conflict of interest.

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