

Hamiltonian-Guided Design of Artificial Molecular Recognition for Multidimensional Chemical Information Transfer

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Modern monitoring systems increasingly demand the ability to transform complex chemical and biological phenomena into actionable information by quantitatively decoding multidimensional chemical information generated by diverse species ranging from ions and reactive molecules to metabolites, lipids, proteins, and cells. Meeting this challenge requires molecular recognition interfaces that are not only highly selective but also programmable, scalable, and adaptable across an ever-expanding chemical space. Conventional biological receptors, however, remain constrained by limited structural diversity, narrow operating windows, and poor designability. In this talk, I will introduce a Hamiltonian-guided framework for engineering artificial molecular recognition using near-infrared fluorescent single-walled carbon nanotubes functionalized with programmable polymer-based corona phases as a universal sensing platform. I will show how this framework enables the rational inverse design of molecular recognition interfaces capable of quantitative monitoring of chemically diverse molecular species with nanometer-scale molecular sensitivity, millisecond temporal resolution, and high spatiotemporal fidelity. By integrating programmable molecular recognition with optoelectronic nanomaterials, sensing instrumentation, computational modeling, and artificial intelligence, I will demonstrate how a common design philosophy can be translated across hierarchical systems ranging from single-molecule interactions and label-free single-cell analysis to early disease diagnostics and continuous online monitoring of complex biological and industrial processes. Beyond individual sensing applications, this talk presents an end-to-end workflow for intelligent sensor development, spanning molecular recognition, signal transduction, hardware integration, multidimensional chemical information transfer, and data-driven decision making. Collectively, this work establishes Hamiltonian-guided molecular recognition as a universal design paradigm for next-generation intelligent sensing systems, bridging molecular interface engineering with programmable chemical information processing.

Keywords: Hamiltonian, corona phase, artificial molecular recognition, sensor, SWCNT, nIR

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