Quantum-Inspired Design of Multi-Functional Nanomaterials for

Simultaneous Imaging, Diagnosis, and Therapy (Theranostics)

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***Abstract*—The integration of imaging, diagnosis, and therapy into unified theranostic platforms has become a central objective in next-generation nanomedicine. However, the design of multifunctional nanomaterials capable of performing these tasks efficiently remains limited by the complexity of nanoscale interactions, nonlinear structure–property relationships, and the combinatorial nature of material optimization. This study explores a quantum-inspired computational framework for guiding the design of theranostic nanomaterials, leveraging quantum-inspired annealing, tensor network representations, and high-dimensional optimization inspired by quantum mechanics. By applying these techniques, the framework accelerates the discovery of optimal nanostructures, surface chemistries, and functional moieties for enhanced contrast imaging, targeted drug delivery, photothermal and photodynamic therapy, and real-time diagnostic monitoring. Simulation-based experiments demonstrate that quantum-inspired methods outperform classical heuristics in identifying candidate materials with superior energy absorption, signal-to-noise ratios, and therapeutic precision. The results highlight the transformative potential of quantum-inspired design for advancing multifunctional theranostic systems, enabling personalized, high-efficiency medical interventions.**

Theranostic nanomaterials—engineered platforms capable of simultaneous imaging, diagnosis, and therapy—represent one of the most promising frontiers in modern biomedical engineering [3]. By integrating multiple functional capabilities into a single nanoscale construct, theranostic systems aim to improve diagnostic accuracy, enhance treatment specificity, and reduce systemic toxicity [5]. Applications range from cancer therapy to neurological imaging, gene delivery, and real-time disease monitoring. Despite these advances, designing nanomaterials with synergistic optical, magnetic, chemical, and biological properties remains a significant scientific challenge. Traditional design strategies rely heavily on trial-and-error experimentation or classical computational heuristics, which often struggle to explore the vast combinatorial design spaces associated with nanoscale systems [7].

Quantum-inspired computation offers a compelling alternative. Unlike quantum computing, which depends on physical qubits, quantum-inspired approaches emulate quantum mechanisms—such as tunneling, entanglement-like correlations, and high-dimensional tensor representations—on classical hardware [4]. These algorithms excel at navigating rugged optimization landscapes and discovering complex structure–property relationships, making them ideal for nanomaterial design. Quantum-inspired annealing,

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