【Grant-in-Aid for Transformative Research Areas（A）】

Photokineticism: Multiscale Kinetics of Excited States and Innovative Optical Functions

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Project Information	Project Number : 26A201　Project Period (FY) : 2026-2030 Keywords : Rate constant prediction, Excited-state dynamics, Spatiotemporal multi-scale, Amorphous aggregates

Purpose and Background of the Research

●Outline of the Research

Many natural phenomena arise from multiple elementary processes that occur sequentially and competitively beneath a single observable event. Experiments usually capture only the macroscopic outcome of all these processes combined, whereas theoretical and computational studies have typically focused on only a subset. A true understanding, however, requires elucidating both the individual elementary processes and the holistic picture that integrates them.

In this context, we have recently developed a quantum chemical methodology for organic molecules that quantitatively and comprehensively predicts overall emission behavior from its constituent elementary processes (*Nat. Commun.* 2024, *15*, 4723). At the same time, we are developing experimental techniques to quantitatively observe previously unexplored “invisible processes,” in addition to the well-studied “visible” ones (*J. Phys. Chem. Lett.* 2019, *10*, 2475). By integrating these computational and experimental approaches with the rate constant as a unifying metric, complex real-world photophysical phenomena can be understood in a unified and quantitative manner from their elementary processes.

Drawing an analogy to kineticism in art—a technique of decomposing a whole into rhythmic elements for pictorial construction—we term this emerging research area “Photokineticism,” denoting a discipline of kinetics centered on light. We will extend our investigations from single-molecule systems to those with intermolecular interactions and, ultimately, to heterogeneous (amorphous) aggregated systems, thereby achieving a fundamental understanding of their spatiotemporal evolution.

This framework promises essential insights into diverse phenomena, quantitative prediction without the need for exhaustive experimentation, and accelerated discovery of novel materials, bringing transformative innovation to every field to which it is applied.

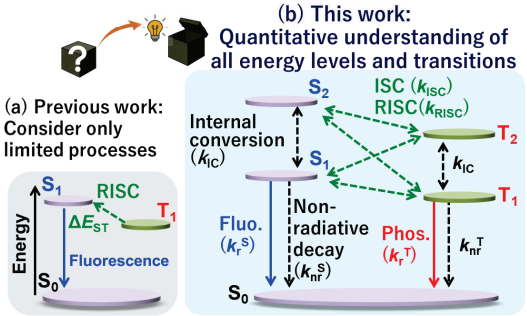

Figure 1. Concept of this research area. By quantitatively determining the rate constants and quantum yields of all elementary processes, we elucidate the essential mechanisms of phenomena that have so far remained “black boxes,” thereby establishing the academic framework of Photokineticism and enabling the development of innovative functions.

Expected Research Achievements

●Research Development of This Area

This research area aims to establish reliable methods for predicting rate constants, which underpin organic photochemistry and many related fields, and to reconstruct their principles from electronic-level elementary processes. In this way, we provide a microscopic basis for macroscopic physical properties and connect quantum-chemical descriptions directly to experiments. Three groups—A01 (design and calculation), A02 (measurement and analysis), and A03 (function)—will work together on the following four subjects to build the scientific foundation of Photokineticism and explore its functional applications.

Rate-Constant Prediction Methods: We will advance our pioneering prediction methodology by fully incorporating vibrational effects and explicitly treating intermolecular interactions in amorphous and heterogeneous systems. In parallel, we will develop experimental techniques to determine rate constants that have been difficult to access, including those of higher excited states and nonradiative pathways, enabling quantitative analysis and validation of excited-state dynamics.

Emission Functions: We will tackle the two major unresolved challenges in OLEDs—efficiency roll-off at high luminance and limited device lifetime—through integrated molecular design, photophysical analysis, and device engineering. By predicting and controlling all relevant rate constants and excited-state processes in a unified framework, we aim to clarify the mechanisms responsible for roll-off and degradation and to propose designs that realize high efficiency, high brightness, and long operational stability.

Photochemical-Reaction Functions: We will extend our methodology from emission to photochemical reaction systems, focusing on photocatalysts that operate selectively in complex environments, such as those that suppress amyloid β aggregation only in the presence of the peptide. By clarifying the origin of such on–off behavior at the level of elementary processes, we will guide the rational design of more advanced photocatalysts with high selectivity and efficiency.

Photoinduced Spin Functions: Building on our studies of singlet fission dynamics, room-temperature quantum coherence, and the modulation of photoinduced spin functions by chiral assembly in metal–organic frameworks, we will explore the relationships between structure, spin states, and dynamics. By controlling molecular packing, framework topology, and chirality, we will manipulate polarized electron spins, their quantum coherence, and the associated rate constants to develop quantum sensing materials for precise temperature and magnetic-field monitoring.

In summary, by integrating theory, computation, and measurement to describe entire phenomena from their elementary processes—across multiscale space (from single molecules to aggregates) and broad timescales—we enable quantitative prediction of whole systems. Beyond luminescent materials and devices, we will broadly apply this foundation, further advancing the Photokineticism framework and developing diverse functionalities.

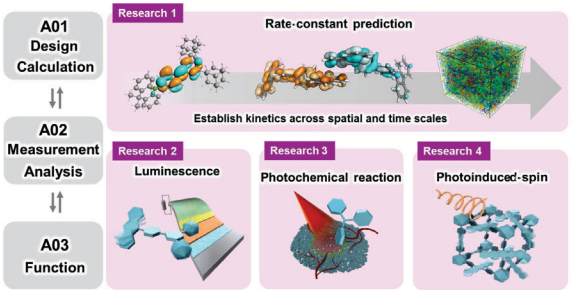

Figure 2. Organizational chart. The research framework A01–A03 (vertical) and Area Tasks 1–4 (horizontal) jointly drive the theoretical and functional development of Photokineticism.

Website(s)	https://pkism.jp