

Advanced Inorganic Synthesis Seminar 2026

Counting photons where chemistry happens: from LDOS engineering to photocatalytic rate constants

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Place : N-531C (Uji Main Building)

Abstract

Photons drive luminescence and photocatalysis only where they actually meet an emitter or a catalytic site. Nanostructures are routinely claimed to “enhance” both processes, yet the step from an electromagnetic calculation to a measured rate constant is rarely taken quantitatively. This seminar presents a single strategy applied to three families of materials: compute a physically controlled optical quantity — the local density of optical states (LDOS), the near field, or the internal photon fluence — couple it to a kinetic model, and confront the result with several experimental observables at once.

(i) Engineering emission. Ta₂O₅-coated colloidal microsphere lattices tune their photonic resonance over ~80nm through shell thickness alone and enhance Rhodamine 6G fluorescence; an emitter-placement model grounded in capillary wetting reproduces the measured Purcell factors. A corrugated Au/Al₂O₃ grating accelerates the red Er³⁺ emission of upconversion nanoparticles by ~15% while leaving the green band untouched, and a coupled FDTD/rate-equation framework reproduces the red-band behaviour while identifying, by elimination, what it cannot explain.

(ii) Counting photons in porous photocatalysts. Compact diffusion-theory scaling laws link transport mean free path, surface-to-volume ratio and thickness to intrinsic rate constants of TiO₂/SiO₂ monoliths. Three-dimensional Monte Carlo transport through Cahn–Hilliard spinodal aerogels then shows that the catalytic solid receives 50–77% more photons than the volume average suggests, biasing extracted kinetic descriptors by up to a factor of 1.9.

(iii) Designing for hot carriers. In an ongoing project, a superlattice of covellite CuS nanoplates is designed for cooperative near-infrared hot-carrier photocatalysis; computational screening predicts a modest ~2× gain at 1064 nm together with a built-in negative control at 808 nm.

Throughout, the emphasis is on where the models succeed, where they fail, and what those failures teach the chemist designing the next material.

Work in collaboration with R. Backov, S. Ravaine (CRPP), X. Liu (NUS Singapore), A. Mihi (ICMAB Barcelona), C. Farcău (INCDTIM Cluj-Napoca), T. Teranishi (Kyoto University) and J. Onoe (Nagoya University).

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