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Plasmonic Nanoparticle–Aerogel Hybrid Photocatalysts for Enhanced Light Harvesting and Gas–Phase Photoredox in Flow Systems

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ABSTRACT

Silica and titania aerogels incorporating plasmonic metal nanoparticles represent a class of highly porous photocatalytic materials for light-driven gas–phase reactions in flow systems. These hybrid materials combine the strong optical response of plasmonic nanostructures with the high surface area, transparency, and tunable refractive index of aerogels, enabling enhanced light harvesting, efficient mass transport, and improved catalytic performance. This work presents a combined computational and experimental approach to the design of plasmonic nanoparticle–aerogel photocatalysts. Electronic-structure calculations based on density functional theory (DFT) are used to determine dielectric properties, which are subsequently implemented in finite-difference time-domain (FDTD) simulations to analyze photon transport, light trapping, and near-field enhancement in three-dimensional porous networks. The simulations reveal that low-index silica aerogels promote broadband visible-light scattering, whereas higher-index titania-containing matrices induce stronger electromagnetic field confinement and red-shifted localized surface plasmon resonances. Enhanced electromagnetic hot spots are localized at nanoparticle–pore interfaces, highlighting the role of pore morphology and refractive-index gradients in controlling photocatalytic activity. Guided by these insights, transparent monolithic aerogels were synthesized using a modified sol–gel method with methyltrimethoxysilane (MTMS) and titania co-precursors, followed by supercritical CO_2 drying. Plasmonic nanoparticles were incorporated in situ to achieve uniform dispersion while preserving high optical transparency. Structural and optical characterization confirmed the formation of homogeneous aerogel networks with tunable porosity and favorable light-scattering properties. Ongoing work focuses on evaluating charge-carrier dynamics and photocatalytic performance under simulated solar irradiation, including gas–phase photoreforming reactions for hydrogen production. The results establish a predictive framework linking aerogel structure, optical response, and catalytic function, providing design guidelines for scalable plasmonic photocatalysts in continuous-flow reactors for sustainable energy applications.

KEY WORDS

plasmonic photocatalysis; aerogels; light trapping; FDTD; flow reactors; energy conversion

BIOGRAPHY

Dr. Kamil Czelej is a researcher and project manager at the Faculty of Chemical and Process Engineering, Warsaw University of Technology. His work focuses on computational materials science, plasmonic nanostructures, and energy-related applications, including photocatalysis and hydrogen technologies. He has authored over 25 publications in international journals and is co-inventor of multiple patents in advanced materials and clean energy systems. Dr. Czelej is a co-founder of the deep-tech company HIPERH2, developing high-performance hydrogen production technologies. He has led and managed national R&D projects and collaborates with academia and industry on translating innovative materials solutions into practical applications.

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