MXenes as Versatile 2D materials for Photocatalysis

Ana Primo, Hermenegildo García
Instituto de Tecnología Química (CSIC-UPV) Avda/ Los Naranjos s/n 46023 Valencia, Spain
aprimoar@itq.upv.es

MXenes have emerged as a unique class of 2D transition metal carbides and nitrides combining metallic conductivity, tunable surface chemistry, and strong light–heat conversion capability. While initially explored for energy storage, their potential as active platforms for photocatalysis is only beginning to unfold. Here we present a coherent research framework demonstrating how MXenes can be engineered across multiple length scales, from quantum dots to heterostructured interfaces, to control charge dynamics and reaction pathways in solar fuel production.

At the nanoscale, we developed a green, HF-free laser ablation strategy to produce MXene quantum dots directly from MAX phases.[1] Quantum confinement and surface functionalization[2] transform metallic MXenes into semiconducting nanostructures with tunable band gaps and visible-light-driven hydrogen evolution activity, establishing size reduction as a viable strategy to activate MXenes photocatalytically.

At the interface level, we constructed 2D/2D MOF–MXene Schottky junctions that prolong carrier lifetimes through interfacial electronic coupling.[3] The intimate van der Waals contact between atomically thin components enables directional charge separation, demonstrating that MXenes can act not merely as conductive supports but as active electronic partners in heterostructures. Moving beyond charge separation, we recently demonstrated that MXene-based Ni heterojunctions operate through an S-scheme charge transfer mechanism under photothermal conditions.[4] In this architecture, surface-state evolution at Ni–NiOx/MXene interfaces governs CO_2 hydrogenation selectivity between CH_4 and CH_3OH. Operando spectroscopy and DFT calculations reveal that catalytic behavior is dictated not simply by oxidation degree, but by dynamic surface-state regulation that modulates adsorption energetics and reaction barriers.

Collectively, these studies establish MXenes as versatile 2D photocatalytic platforms in which activity and selectivity can be rationally tuned via (i) quantum confinement, (ii) 2D/2D interfacial engineering, and (iii) surface-state control under operational conditions. This multiscale approach positions MXenes as powerful building blocks for next-generation solar fuel technologies.

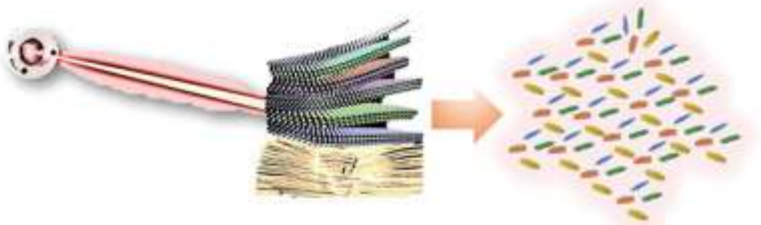

Figure 1: Insert caption to place caption below figure (Century Gothic 10)

References

[1] Rubén Ramirez-Grau et al., Small methods, 7 (2023), 2300063
[2] Rubén Ramirez-Grau et al., Appl. Catal. B: Environ., 341 (2024), 123316
[3] María Cabrero-Antonino et al., Angew. Chem. Int. Ed.,64, (2025), e202503860
[4] Dawid D. Kruger et al., Angew. Chem. Int. Ed. (2026), e8425918,