Investigation of the effects of nanoscale facets on catalytic activity in photo-driven nanosystems

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Nanoparticles exhibit extraordinary catalytic activity due to their high surface area, tunable morphology, and unique electronic properties. Among these, facets and surface defects play a pivotal role in enhancing photocatalytic reactions. In this study, we aim to unravel the nanoscale mechanisms governing charge-driven photocatalytic processes on single, isolated nanoparticles with varying morphologies. Utilizing a combination of velocity map imaging (VMI) and coherent diffractive imaging (CDI) at the Maloja instrument at SwissFEL, we probe the ultrafast dynamics of spherical and cubic gold nanoparticles (AuNPs) in a time-resolved optical pump and X-ray probe scheme.

Results reveal orientation-dependent ion momentum distributions and enhanced ionic yields correlated with nanoparticle facets. These observations suggest that near-field enhancement effects at high-index facets significantly modulate catalytic activity. By systematically analyzing ionic fragment momenta across varying time delays and nanoparticle orientations, we establish a direct relationship between nanoparticle morphology and site-specific reactivity. The multimodal approach combining VMI and CDI provides unprecedented insight into the role of structural factors in nanoscale photocatalysis, advancing our understanding of clean energy processes and catalysis optimization.

Keywords: Catalysis, nanoparticles, XFEL

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