Energy Conversion in Plasmonic Materials: an Atomistic Perspective

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Most properties of plasmonic nanostructures follow from the tunability of their optical response as a function of their shape and dimensions [1] The accurate description of the optical properties of the plasmonic substrates is crucial for rationalizing the physical phenomena occurring at the plasmon resonance frequency [2]. In this context, an in-depth understanding of the dynamics of the optical response of plasmonic structures is vital for elucidating the mechanisms underlying the photophysics, photochemistry, and catalytic activity of such systems, which are intrinsically connected with the huge amount of energy absorbed by plasmonic materials [3-4].

Here, we present a novel theoretical approach explicitly defined in the real-time domain, based on a fully atomistic description of the nanostructure to describe the plasmon dynamics of complex materials [5]. The method effectively captures quantum size effects in metal nanoparticles, including plasmon shifts in simple and d-metals, even below the quantum size limit [6-8]. The developed realtime formulation provides a robust framework for exploring the time-dependent optical behavior of metal nanostructures, such as the decoherence of plasmon excitations, closely tied to their potential applications in photochemistry, and photoreactivity.

Our approach serves as a comprehensive and efficient tool for studying the optical response dynamics in metal nanostructures, bridging classical and quantum descriptions, and paving the way for advanced applications in photonics, plasmonics, and catalysis.

References

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