

Smart Nanohybrids and Multi-Material Nanoparticles: Synthesis, Properties, Modeling and Applications

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Abstract:

Many applications of modern nanotechnology take advantage of various properties of smart nanomaterials, such as optical, thermo-, mechano-, magneto-plasmonics, etc., where one property is enhanced or modified due to another [1-3]. Thus, nanoparticle aggregation and fragmentation, formation of bi-metallic, multi-material, alloy, Janus, and/or multi-component nanoparticles pave the way toward extremely wide modification possibilities of their absorption spectra, but also of their physical properties and potential functions in various fields including medicine, solar energy, catalysis, etc.

Ultra-short laser pulses are, furthermore, extremely versatile tools well-suitable for nanoparticle generation and for the following modifications of their sizes, shape, composition, and morphology [2]. Laser absorption and scattering effects rely on their plasmonic properties, but also on their band structure, size, composition, shape, and concentration as well as on the main laser parameters, such as wavelength, intensity, and pulse duration. The following laser-induced phenomena include electronic processes, fast heating, chemical reorganizations, various phase transitions, sintering and/or decomposition, as well as longer relaxation and cooling. Atomistic approaches, such as all-atom molecular dynamics simulations are particularly advantageous for numerical modeling of such systems.

In this study, several examples of laser-induced modifications of smart nano-hybrids, nano-alloys, and multi-material nanoparticles will be presented. Firstly, attention is focused on the initial heating stage accompanied by melting, sintering and/or fragmentation. Then, the cooling is addressed, where phase and species segregation and annealing take place. Size- and composition-dependent particle modifications are thus examined. The obtained results are of interest for the analysis of pulsed laser-induced nanoparticle formation in liquids (PLAL) [1-3], nanoparticle aggregation-fragmentation experiments, sintering, 3D manufacturing, etc.

Particularly, bimetallic nanoparticles, such as AgAu, AlAu, CoAu, and FeAu, CoNi are to be

considered. Then, attention is focused on more complex nanoformulations, such as raspberry or core-shell Ni@Au, Au@Ni, Co@Au and Au@Co, Fe@Au and their oxides, their structure, optical, magnetic, and chemical properties, as well as their interests for applications such as cancer theranostics and photocatalysis.

Keywords: femtosecond laser, molecular dynamics, smart nanohybrids, alloys, catalysis, cancer theranostics, solar cells.

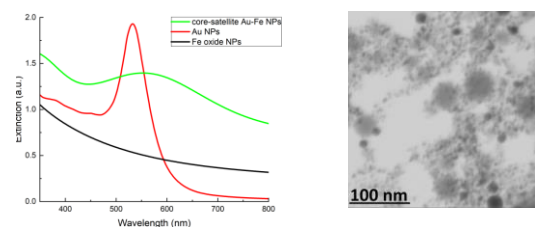


Figure 1: Calculated extinction spectra of bare Au NPs (red line), Fe oxide NPs (black line) and core-satellite Au-Fe NPs (green line) and image of nanostructures formed from laser-ablated Au NPs and Fe NPs in liquids.

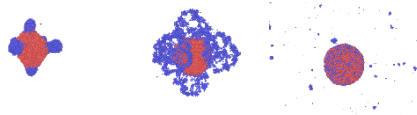


Figure 2: MD simulations of Ni@Au and Au@Ni nanoformulations after laser heating in different regimes.

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