

THEORETICAL STUDY OF BIMETALLIC PLASMONIC NANOSTARS AND THEIR EFFICIENCY AS PHOTOCATALYSTS

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Nanostars (NSs) provide a very promising template for the study of plasmonic-enhanced processes, in particular driving photocatalytic reactions, due to their intense hot-spots, which are combined with a quasi-spherical symmetry that separates them from plasmonic nanorods [1]. It is still an open question, however, how to best exploit these nanostructures in different specific applications, as their response is very sensitive to small changes in their properties, and using this geometry in multimetallic systems, which have shown great promise in the past, [2] further expands the space of possibilities.

We present a work in which we have precisely explored how multimetallic NSs respond in a photocatalytic context. We have performed a computational study of the optical response of different NSs made of gold and silver, modelling bimetallic NSs grown experimentally. Our theoretical approach allows us to study the expected relative importance of different energy transfer mechanisms between plasmonic NS and environment to the photocatalytic process. With these results, we can critically evaluate the expected photocatalytic outcomes of using silver-coated and uncoated gold NSs. We also studied the reverse system, gold-coated silver NSs, with the same geometries, to offer a comprehensive discussion of the use of multimetallic systems in photocatalytic applications.

- Sousa-Castillo, A., Comesaña-Hermo, M. & Rodríguez-González, B. et al. The Journal of Physical Chemistry C 120, 21 (2016), 11690-11699.
- [2] Negrín-Montecelo, Y., Comesaña-Hermo, M., Khosravi Khorashad, L., Sousa-Castillo, A. & Correa-Duarte, M.A. et al. ACS Energy Letters 5, 2 (2020), 395-402.



Figure 1: Schematic representation of a transverse cut at the center of the nanostars studied in this work. Left: Aucore@Ag-shell nanostar. Right: Ag-core@Au-shell nanostar.