Modelling plasmo-catalytic solar energy conversion

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Abstract: Metallic nanoparticles are efficient absorbers of sunlight because of the large dipole moment of localized surface plasmons (LSP). Hot electrons and holes generated from the decay of the LSP decay can be harnessed to trigger chemical reactions or generate a electric current, but a detailed understanding of the fundamental processes of such nanoplasmonic hot carrier devices is currently lacking. To address this problem, my group has developed new material-specific methods to model the dependence of hot carrier properties on the size, material composition and environment of the nanoparticle [1]. I will also present results for bimetallic core-shell nanoparticles for water splitting applications and discuss which combinations of metals yields optimal performance [2].

References:

[1] Dal Forno, Ranno, Lischner, *J. Phys. Chem. C*, **2018**, *122*, 8517.

[2] Ranno, Dal Forno, Lischner, *npl Computational Materials*, **2018**, *4*, 31.

Biography: Johannes Lischner currently a Senior Lecturer and a Royal Society University Research Fellow in the Department of Materials at Imperial College London.

He obtained a Ph.D. in theoretical physics from Cornell University in 2010 working in the group of Prof. Tomas Arias. From 2010 to 2014, he was a postdoctoral researcher at UC Berkeley and Lawrence Berkeley National Lab in the groups of Prof. Steven Louie and Prof. Marvin Cohen.

In his research, Johannes studies the physical and chemical properties of materials using theoretical modelling approaches. Currently, much of my work is focused on nanomaterials and energy materials. For example, he is interested in understanding the properties of twisted bilayer materials, catalytic metal surfaces, plasmonic nanoparticles and defects. To learn about the properties of these materials, he employs a variety of modelling techniques ranging from quantum-mechanical approaches, such as many-body perturbation theory (GW/BSE method) or density-functional theory, to classical force fields and elastic continuum models.