Exploring Plasmon Decay in Metallic Nanoparticles with Time-Dependent DFTB

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Since 2016, we have been studying plasmon decay mechanisms in metallic nanoparticles using the Time-Dependent Density Functional Tight Binding (TD-DFTB) method. This presentation will share our findings and also highlight the areas that need further research. The TD-DFTB approach, with its balance between computational cost and model accuracy, has been crucial in our research, a subject that will be expanded upon by other speakers in this workshop.

We will discuss our research results, from understanding how different metals behave during electronic relaxation, the impact of surface chemistry on these processes, to the possibility of using hot electrons from plasmon decay to trigger highly endothermic chemical reactions. This last point is particularly interesting for the potential use of composite metal-metal oxide nano-structures as photo-catalysts.

Our presentation will summarize and communicate the key findings from a series of papers that we have published on this topic. These papers cover a range of areas, including chemical interface damping of surface plasmon excitations in silver nanoclusters [1], differences in energy absorption in gold and silver nanoclusters [3], the dynamics of hot carrier generation in these nanoparticles [4], and the role of the dynamic Schottky barrier in stabilizing electron-hole pairs for photocatalysis [5].

Our goal is to provide a clear and accessible understanding of plasmon decay and hot carrier dynamics, and we hope that our work will help to stimulate further research in this important field [6].

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[6] C. G. Snchez and M. Berdakin, J Phys Chem C 126, 10015 (2022).