Multiscale Screening of Plasmon Enhanced Photocatalysts

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Metallic nanoalloys (NAs) have long been studied for their vast array of promising, novel applications, from biosensors to photovoltaics. Here, we are particularly interested in the plasmon enhanced photocatalytic properties of NAs, combining a plasmonic (gold) and a catalytic (platinum) material for their potential application in plasmon enhanced photo-catalysis [1]. Great attention has been paid to the development of such devices as the utilisation of localised surface plasmon resonances (LSPRs) has proven itself a viable and sustainable means of generating kinetically active electrons and holes for photo-catalytic reactions [2].

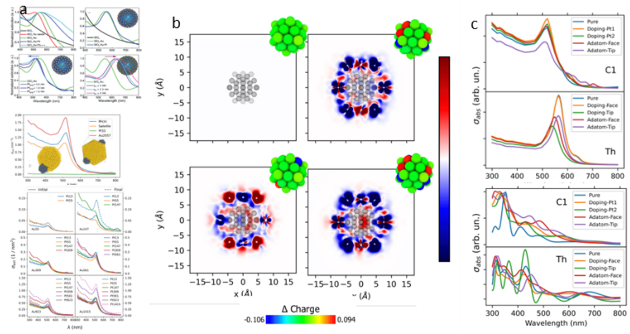

Figure 1: **a.** Comparison between experimental results from [3] and the classical model. **b.** Time evolution of the induced electronic dipole subject to optical stimulation. **c.** Comparison of extinction spectra evaluated from classical (top) and ab initio (bottom) approaches for small NAs taken from [4]

In this talk, we shall look to recent experiments to instruct a design philosophy [3], adopting morphologies of small Pt decorations upon a larger Au seed, and core-shell NAs. This, in principle, ensures that the adsorption surface provided by the Pt is supported atop a larger Au nanoparticle. We shall present the findings of recent investigations into a the stability of composite nanoclusters where the relative alloy ratio of AuPt NAs is varied, and the classically predicted photo-extinction spectra for the corresponding morphologies. We shall also report on the structure – properties relationship of small AuPt NAs wherein we consider both the static electronic properties, and the photo-absorption spectra to determine plasmocatalytic efficacy [4]. We present in Figure 1 the key results from these recent investigations.

References

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