Strain-dependent electronic and optical properties of metals for photocatalytic applications

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Photocatalytic production of hydrogen fuel from untreated sources of water is one of the highly sought methods for solar-to-fuel conversion, mainly due to its higher power density, ease of storage and transportation, and the possibility to ameliorate the intermittent nature of solar energy. However, photocatalytic systems performance ($< 10\%$) has been hindered due to the poor absorption of visible light on wide band gap oxides.

Recently, it has been shown that photo-excited hot carriers produced by surface plasmons can be used to carry out highly energetic chemical reactions, or used in photo -voltaic and -electrochemical devices through their transfer into a semiconductor. Initial charge-carriers distributions generated by plasmon decay are heavily dependent on the electronic structure of the metals, and particularly through interband transitions (affecting those involving d-bands) that dominate at higher plasmon energies.
Here, we use a band-structure engineering approach on a series of prototypical noble metals and other metal alloys under various values of strain. Electronic structure and optical properties are analysed to determine changing features and their origin, and their possible impact on the initial charge-carrier densities at different electron excitation energies —including those related to decay of surface plasmons. We will discuss our results in terms of carriers distributions for different materials and strain conditions, and will hint design principles for enhanced hot-carriers generation.

[*] This work was funded under the Cooperative Agreement between the Masdar Institute of Science and Technology, Abu Dhabi, UAE and the Massachusetts Institute of Technology, Cambridge, MA, USA, Reference Number 02/MI/MIT/CP/11/07633/GEN/G/00.