# Optical properties, transport and sensing in metal-molecular aggregate hybrid nanostructures

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**Abstract**

Following the emerging connection between the fields of molecular electronics and plasmonics, we have studied theoretically the optical properties of gold nanoparticle (NP) dimers linked by a molecular bridge [1,2]. In a first approach, we have modelled the linker as a pure conductor with real conductivity. The main resonances governing the optical spectrum are the Bonding Dimer Plasmon (BDP), the Screened BDP (SBDP) and the Charge Transfer Plasmon (CTP) modes, depending on the conductance through the linker. The BDP and the SBDP modes arise from the hybridization of the dipolar modes of the individual NPs, whereas the CTP resonance involves a net current through the junction. This simple model allows us to establish thresholds of conductance for the activation of the SBDP and CTP modes, indicating when the transport through the linker starts to affect the optical properties of the dimer.

In a second step, we have incorporated the excitations of the individual molecules by introducing a Drude-Lorentz model for the dielectric response of the linker [3]. In this case, the BDP and the Bonding Quadrupolar Plasmon (BQP) resonances, with the BQP arising from the hybridization of the quadrupolar modes of the individual NPs, couple to the molecular excitonic transition. In spite of the complexity introduced in the dielectric response, we find that the concept of conductance threshold for the emergence of the CTP mode previously introduced for metallic linkers is still valid. We have performed a deep analysis of the effects of the excitation energy and the density of the molecular aggregates on the optical spectroscopy of the hybrid structures.

Finally, we have explored the efficiency of the new mixed states for LSPR sensing, showing that the CTP mode is a good candidate for shift-based sensing. Furthermore, for the BDP-exciton mixed states, we have observed an interesting behaviour for sensing based on the change of the relative intensity of the resonances, thus introducing a new framework for sensing based on the evolution of plexcitonic intensities rather than on spectral shifts.

**References**

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