# The quantum regime in tunneling plasmonics

**J. Aizpurua**[1], R. Esteban[1] , A. G. Borisov[2], P. Nordlander[3], K. J. Savage[4], M. M. Hawkeye[4] and J. J. Baumberg[4]

[1]Material Physics Center CSIC-UPV/EHU and Donostia International Physics Center DIPC, Donostia-San Sebastián Spain, ruben_esteban@ehu.es, aizpurua@ehu.es.
[2]Institut des Sciences Moléculaires d'Orsay - UMR 8214, CNRS-Université Paris Sud, Orsay Cedex, France.
[3]Department of Physics,MS61, Laboratory for Nanophotonics, Rice University, Houston, Texas, USA.
[4]Nanophotonics Centre, Cavendish Laboratory, University of Cambridge, Cambridge, United Kingdom
aizpurua@ehu.es

## Abstract

Electron transfer due to quantum tunnelling between two metallic structures strongly modifies the plasmonic resonances of the system. For small particles, the resulting optical behaviour can be studied using Time-Dependent Density Functional Theory (TDDFT) [1]. The particles used in typical plasmonics applications, however, often have dimensions that are tens, hundreds of even thousands of nanometers long, and thus they are too large to be treated with state-of-the-art TDDFT.

Here, we present a Quantum Corrected Model (QCM) that includes the effect of quantum tunnelling in the calculation of the plasmonic response of large structures at subnanometer separation distances [2]. The model requires to define an effective material in the region where tunnelling is happening, with the properties of the material given by exact quantum calculations from a simplified system. A standard solver of Maxwell equations can then be used to obtain the response of the entire system. QCM is straightforward to implement for arbitrary geometries, which can exhibit narrow gaps or particles in contact.

We first test the QCM results against small Na spheres that can be also simulated using TDDFT, and find very good agreement between both methods. Next, we consider the case of large Drude-like Au structures to illustrate the effect of tunnelling in realistic plasmonic systems formed by large nanometric structures. As expected from previous work in small particles, we observe a spectral redistribution of the modes for all the geometries and a collapse of the near-field enhancement at very short separation distances..

We also consider the experimental situation of two approaching gold tips, a system which we have recently tested to experimentally reveal quantum effects in plasmonic gaps at subnanometer separation distances [3]. The modelled structures (longer than 1 micrometer), exceed by several orders of magnitude the sizes typically tackled with TDDFT. Notably, the measured and calculated far-field spectra are in good agreement, which further emphasizes the relevance of the proposed method to correctly address experimental situations. Moreover, our QCM simulations open the possibility to predict both the optimal near field enhancement and confinement expected a task that has still not been yet reported experimentally.

## References

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