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Optical response of metal nanojunctions driven by single atom motion: influence of quantized electron transport on nanoplasmonics[1]

DANIEL SANCHEZ-PORTAL, FEDERICO MARCHESIN, Centro de Fsica de Materiales de San Sebastin CSIC-UPV/EHU and DIPC, Spain, PETER KOVAL, Donostia International Physics Center (DIPC), Spain, MARC BARBRY, JAVIER AIZPURUA, Centro de Fsica de Materiales de San Sebastin CSIC-UPV/EHU and DIPC, Spain — The correlation between transport properties across sub-nanometric metallic gaps and the optical response of the system is a complex effect that, similarly to the near-field enhancement [1], is determined by fine atomic-scale details in the junction structure. Using ab initio calculations, we present here a study of the simultaneous evolution of the structure and the optical response of a plasmonic junction as the two $Na_{\{}380$ clusters forming the cavity approach and retract. Atomic reorganizations are responsible for a large hysteresis of the optical response. The system exhibits a jump-to-contact instability during the approach, and the formation of an atom-sized neck across the junction during retraction. Due to the quantization of the conductance in metal nanocontacts, atomic-scale reconfigurations play a crucial role in determining the optical response. We observe abrupt changes in the intensities and spectral positions of the dominating plasmon resonances, and find a one-to-one correspondence between these jumps and those of the quantized transport across the neck. These results point out to an unforeseen connection between transport and optics at the atomic scale, which is at the frontier of current optoelectronics. [1] M. Barbry, et al., Nano Letters 354, 216 (2015)

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