Characterizing plasmons at the nanoscale by first-principle simulations

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First principle methods such as time-dependent density functional theory are becoming increasingly popular in the investigation of surface plasmons localized on metallic nanoparticles and non-conventional plasmonic materials such as graphene nanoflakes. Besides revealing the dependence of the plasmon excitations on the microscopic details of the systems (atomistic geometry, role of surfactants and of the environment, etc.), such methods can also address basic questions such as the fundamental (quantum) nature of the plasmonic excitations themselves. In fact, nanoparticles are composed of electrons and nuclei like ordinary molecules. Therefore, it should be possible to understand their excited states, including plasmons, in terms of the same elementary electron-hole excitations routinely used to interpret molecular excited states, and to find the microscopic features that distinguish plasmonic from non-plasmonic excitations. In this talk I will present possible approaches to address this important problem, and the related results obtained so far by our group [1-3].

References

[1] L. Bursi, A. Calzolari, S. Corni, E. Molinari, ACS Photonics **1**, 1049 (2014);
[2] L. Bursi, A. Calzolari, S. Corni, E. Molinari, ACS Photonics **3**, 520 (2016).
[3] R. Zhang, L. Bursi, J. D. Cox, Y. Cui, C. M. Krauter, A. Alabastri, A. Manjavacas, A. Calzolari, S. Corni, E. Molinari, E. A. Carter, F. J. García De Abajo, H. Zhang, and P. Nordlander, ACS Nano **11**, 7321 (2017).