Carl von Ossietzky
Universität
Oldenburg
Institut für PHYSIK

PHYSICAL COLLOQUIUM

INVITATION

Monday, 17.01.2022, 4.15 p.m.,
video conference: https://meeting.uol.de/b/anj-2vc-j6s-fwe

speaks

Prof. Dr. Stefano Corni,

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about

"Atomistic modeling of molecular nanoplasmonics: from enhanced spectroscopies to photochemistry in the strong coupling regime"

Localized surface plasmons (LSPs), collective excitations of the conduction electrons in nanostructures, have several outstanding properties, such as large absorption cross sections, shape- and environment-sensitive resonance frequencies, and the capability of enhancing an incident electromagnetic field in their nanoscopic proximity (optical nanoantenna effect). The latter is a precious tool to manipulate light at the nanoscale, being for example the most relevant contribution to surface enhanced and tip enhanced spectroscopies (Raman scattering, vibrational absorption, photoluminescence) of nearby molecules. The electromagnetic field associated to the LSP excitation can be so locally intense to allow entering the plasmon-molecular excitation strong coupling regime, where hybrid excitations can be separately addressed. This profoundly changes the properties of the molecule, including its photochemistry.
In this seminar, I will provide a description of the multiscale modeling approaches we developed through the years to simulate such phenomena, and discuss a few selected systems to show the physics they can disclose. The basic model [1,2], that started as an extension of the Polarizable Continuum Model for solvation of molecules to their proximity to a NanoParticle (PCM-NP), exploits an atomistic quantum approach for the molecule (e.g., DFT and TDDFT) and a description of the nanostructures based on macroscopic electrodynamics. More recently, it has been extended to simulate the time-dependent behavior of the system [3,4] so to treat pulsed light experiments and the related dynamics, making natural the inclusion of dephasing and decoherence effects via a Stochastic Schrödinger Equation (SSE) approach [5].

This also inspired approaches to simulate photochemistry of realistic molecules in the strong coupling regime [6,7], that revealed how important the chemical complexity of the molecule is to understand and to manipulate strong coupling photochemistry. Finally, the modeling also provided a natural way to quantize the LSPs, and to explore how the electronic structure of the molecule, computed at the Coupled Cluster level, is affected in the strong coupling regime[8].

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[2] B. Mennucci, S. Corni; Nat. Rev. Chem. 3, 315 (2019)

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[4] J. Jannis, G. Gil, S. Corni, C. Cocchi; J. Chem. Phys. 154, 224114 (2021)

[5] E. Coccia, F. Troiani, S. Corni; J. Chem. Phys. 148, 204112 (2018)

[6] J. Fregoni, G. Granucci, E. Coccia, M. Persico, S. Corni; Nat. Comm. 9, 4688 (2018)

[7] J. Fregoni, G. Granucci, M. Persico, S Corni; Chem 6, 250 (2020)

[8] J. Fregoni, T.S. Haugland, S. Pipolo, T. Giovannini, H. Koch, S Corni; Nano Lett. 21, 6664 (2021)

All interested persons are cordially invited.

Sgd. Prof. Dr. Caterina Cocchi