Nanostructures & (Bio)molecules Modeling

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The group is developing and applying multiscale computational methods for hybrid systems, such as organic and biological molecules interacting with inorganic nanoparticles. The exploited methods range from ab initio atomistic calculations and classical molecular dynamics to classical electrodynamics. The main research topics are:

- ultrafast spectroscopy and optical properties of molecules close to plasmonic nanostructures & in solution, including surface enhanced optical phenomena. -the quantum nature of plasmonics excitations at the nanoscale.
- the interactions of inorganic surfaces and nanoparticles with proteins.

Currently the group is funded by the ERC CoG Grant TAME-Plasmons (2016-2021), dedicated to develop simulation approaches for the optical properties of molecules close to plasmonic nanostructures.

- *How to Identify Plasmons from the Optical Response of Nanostructures,* ACS Nano, **2017**, 11, 7321–7335.
- *The interaction with gold suppresses fiber-like conformations of the amyloid β (16–22) peptide,* Nanoscale, **2016**, 8, 8737-8748
- *Probing the influence of citrate-capped gold nanoparticles on an amyloidogenic protein,* ACS Nano, **2015**, 9, 2600-2613.
- *Facet selectivity in gold binding peptides: exploiting interfacial water structure,* Chem. Sci., **2015**, 6, 5204-5214.
- *Surface packing determines the redox potential shift of cytochrome c adsorbed on gold,* J. Am. Chem. Soc., **2014**, 136, 12929-12937.