Nanostructures & Biomolecules Modeling

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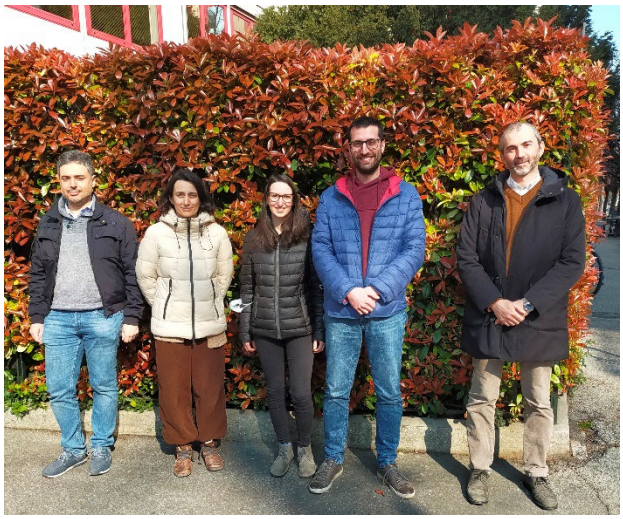

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The group develops and applies multiscale computational methods to describe hybrid systems, such as organic and biological molecules interacting with inorganic nanoparticles. The methods used range from ab initio atomistic calculations (also on quantum computers) and classical molecular dynamics to classical and quantum electrodynamics. The main research topics are:
-ultrafast spectroscopy and optical properties of molecules close to plasmonic nanostructures & in solution.
-the quantum nature of plasmonics excitations at the nanoscale.
-charge and energy transfer in (bio)molecules and in nanoscale structures
-the interactions of inorganic surfaces and nanoparticles with proteins.
The group is currently funded by EU H2020 and HE projects in which light-biomolecule interactions play a major role.

1. *Strong coupling between localized surface plasmons and molecules by coupled cluster theory*, Nano Letters, **2021**, 21, 6664-6670
2. *The physical origin of a photon-number parity effect in cavity quantum electrodynamics,* Results in Physics, **2021**, 30, 104690
3. *Charge transfer between [4Fe4S] proteins and DNA is unidirectional. Implications for biomolecular signaling,* Chem, **2019**, 5, 122-137
4. *Manipulating azobenzene photoisomerization through strong light–molecule coupling,* Nature Communications, **2018**, 9, 4688-9
5. *How to Identify Plasmons from the Optical Response of Nanostructures*, ACS Nano, **2017**, 11, 7321–7335.