Subject 3: **Quantum mechanical and machine learning modelling of aqueous functionalized nanoparticles**

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Molecules on both metallic and molecular nanoparticle surfaces are very challenging systems to accurately model since the large system sizes result in computationally expensive atomistic simulations that are intractable for at least the next decade even on supercomputing platforms.

Artificial Intelligence and machine learning techniques have shown great promise in modeling structure-property relationships and identifying important features from unsupervised learning of atomistic simulations, which may allow one to extend the size and time scales that can be accurately treated. In this project advanced theoretical and computational techniques will be used to model the electronic and optical properties of solvated functionalized nanoparticles that have potential applications in nano-medicine.

Data mining, machine learning and artificial neural networks will be utilized in conjunction with quantum mechanical simulations in order to extract the important underlying information from the large set of electronic structure calculations in order to predict electronic and optical properties of large nanoparticles that are beyond the size that can be quantum mechanically simulated. The neural-network model should accelerate quantum molecular dynamics simulations during the dynamics in order to characterize structural properties, dynamics and the vibrational spectroscopy of the water in the vicinity of the functionalized nanoparticles. This can be used to study the effects ionizing radiation has on nanoparticle systems. This project is relevant to the multidisciplinary research ICP direction ``Ionizing radiation induced elementary processes in biomolecules and nano-objects" and involves experimental and theoretical groups at the ISMO and ICP, respectively. This project will result in a realistic quantum mechanical molecular dynamics description of functionalized nanoparticles solvated in water. This description will permit the interpretation of available optical and spectroscopic experiments that have been performed on nanoparticles (Pt, Gd, Bi…) in the ISMO group. The developed model will provide a deep understanding of the evolution of the plasmonic properties and the charge transfer mechanism that occurs in solvated nanoparticle systems. The results will also be used in subsequent studies of elementary processes induced by external stimuli (ionizing radiation, thermal excitation, light, etc.) that may be of interest for potential medical applications of nanoparticles.

The intern will have the opportunity to participate in the experiments lead by Erika Porcel on the use of nanoparticles for radio-enhancement in radiotherapy. The intern will benefit from the complementary expertise of the theoretical and experimental groups at ICP and ISMO.

Internship duration : 6 months
Your profile: M2 in Medical Physics, M2 SERP or any other M2 interfacing Physics/Chemistry/Biology/Medicine

Gratification : 591.51 €/month
Please apply by sending an email to: erika.porcel@universite-paris-saclay.fr gerard.baldacchino@cea.fr sandrine.dobosz@cea.fr charles.truillet@universite-paris-saclay.fr copy to inanotherad@universite-paris-saclay.fr