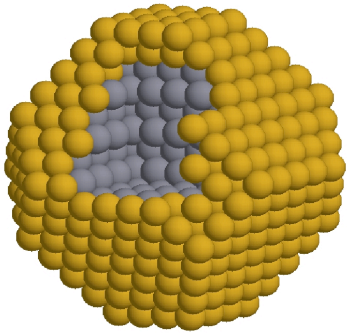
Joint modeling of the structure and the magneto-optical properties of nanoalloys

Directeurs de thèse : Christine Goyhenex and Hervé Bulou
IPCMS-DSI, 23 RUE DU LOESS, BP43, F-67034 STRASBOURG CEDEX 2 (FRANCE)
TEL : 03 88 10 70 97 ; E-MAIL : CHRISTINE.GOYHENEX@IPCMS.UNISTRA.FR

Nanoparticles are widely exploited in numerous domains, like catalysis, medicine and environmental needs. Sensor is an important potential application of the nanoparticles, which relies on the opportunity to couple different properties, in the aim to form a system both sensitive to the external environment and reliable for detection. Magneto-optic biosensors, used in detecting water toxins and contaminants or for diagnostic applications, are some promising examples.

However, designing a suitable sensor requires to set an accurate relationship between the sensor property and the external environment in which evolves the nanoparticle. Nanoalloys[1] (see figure) are a good answer to this problematic since by combining their finite-size effects with the properties of metallic alloys it is possible to exploit the chemical arrangement inside the particle to build coupled multi-property devices. In the nanoalloys, the atomic arrangements (structure and morphology) and the electronic structure should vary with the respective composition of the metals. Controlling the chemical arrangement represents a possible route to tune the magnetic and optical properties, as well as their coupling.

Designing new devices requires to carefully and jointly study structure and properties as a function of the atomic and chemical arrangements of the alloys. The determination of the magneto-optical properties requires to consider the systems at the electronic level, imposing to perform quantum simulations (Density Functional Theory). However, the large involved number of atoms and chemical configurations impose to employ large scales classical simulations as Monte Carlo. The latters will enable to build a phase diagram in which we will select some candidates suitable for chosen targeted properties.



Typical core-shell bimetallic nanoparticle.

The choice of the system to investigate is guided by its ability to combine both magnetic and optical properties. In this context, the weakly miscible materials like AuCo or AgCo are potentially interesting for their magneto-optical properties since they combine a ferro- (Co) and a nonferromagnetic (Au, Ag) metal which presents a sharp surface plasmon resonance. With this model system, we propose, in this thesis, to disentangle the respective roles

[1] Johnston RL (2008) Nanoalloys: from theory to applications of alloy clusters and nanoparticles. Chem Rev 108:845–910. doi:10.1021/cr040090g

of structure, magnetism and optical properties.

The system will be studied by using classical atomistic simulations and density functional theory for the structural and chemical optimization of the systems and the time-dependent density functional theory for determining the magneto-optical properties of the device. A large part of the study will be performed by using centres of intensive numerical calculations such as IDRIS or CINES. Interest in computational physics is recommended for this project.