Helium-mediated Synthesis, Soft-Landing and Spectroscopy of Metal Nanoparticles on Surfaces

Acronym: HeSSSMe 2014

Objective (general)

The Mini-Workshop "Helium-mediated Synthesis, Soft-Landing, and Spectroscopy of Metal Nanoparticles on Surfaces" (HeSSSMe) is intended to bring together theoretical and experimental researchers working in this emerging field of helium droplet research [1-4] as well as researchers who will be interested in future involvements within this area. This meeting is framed within the COST Action CM1200 “Converged Distributed Environment for Computational Spectroscopy” (CoDECS).

Brief History and Motivation

Recent experimental measurements by the group of Vilesov [1] showed that helium droplets can act as carriers for the soft-landing deposition of catalytic metal-nanoparticles, synthesized inside the helium droplets, on the surface of interest. The first theoretical effort aimed to understand this process was accomplished within a joint CoDECS project [2], revealing the key role of nuclear quantum effects within the helium droplet. Related to this topic it is also interesting to see the work by Hinde et al. [3].

During the last two years, interest in helium droplet mediated synthesis/soft-landing has increased considerably so that there are many more experimental groups working in the area [4]. Thus, Ernst's group has investigated the properties of nanoparticles grown inside helium droplets, observing crystallinity [4a], while Lindsay's group has focussed on the formation of metal nanoparticles by helium droplet assembly, demonstrating the level of control that can exist in creating metal cluster-based films [4b]. Also, Ellis' group [4c] has very recently reported on the controlled synthesis of metallic core-shell nano-particles within helium nanodroplets. Experimental studies are currently underway to investigate the electro-, magneto-optical, and catalytic properties of these metal nanoparticles via spectroscopy outside the helium droplet. The microscopic understanding and first-principle simulations of HeSSSMe processes are relevant because they hold the potential to reveal basic mechanistic information and key simplifications.

Description of the Mini-Workshop

The main session of the mini-workshop will be devoted to highlight the problems that might stimulate the development of new (first-principles) methodological strategies and combined experimental/theoretical studies. With this goal, a few experimentalists will be invited to present introductory lectures.

Mainly within the framework of closely related areas, we will discuss about:

1) The Nuclear Motion Problem. The emphasis will be put on computational methods capable of accounting for: (1) the quantum nature of the helium droplet at impact with the surface (e.g., multi-configurational time-dependent Hartree MCTDH and time-dependent density-functional-theory TDDFT); (2) the evolution of the metal nanoparticles after the impact with the surface (e.g., classical and semi-classical treatments including finite-temperature surface effects). Another relevant issue to be discussed is the spectroscopy of the embedded species in situ (inside the droplet) using, e.g., DFT-based [5], path-
integral Monte-Carlo [6], and quantum chemistry-like approaches [7]. Also, the application of the diffusion Monte-Carlo method [8] to metal nanoparticles grown processes, as well as the properties of helium adsorbed on surfaces, will be considered.

2) The Interaction Problem. The aim is to deal accurately with the dispersion-dominated He-surface interaction [9], for example using special techniques that combine full ab-initio calculations on small cluster models with DFT-based treatments of dispersionless correlations effects on larger clusters, including the extension to periodic boundary conditions. Methodologies enabling the partitioning of supermolecular interaction energies in order to device ad hoc functionals will be also considered. The session will also cover the characterization of dispersion interactions within the metal nanoparticles [10]. Likewise, the applicability of embedding techniques for the description of the metal-surface interactions and the many-body effects within the metal nanoparticles, as those applied and/or developed within CoDECS joint projects, e.g. [11], will be debated.

3) The Spectroscopy of the Deposited Metal Nano-particles. CoDECS members interested in the catalytic and magneto-optical-electronic properties of the deposited metal nano-particles will be invited to participate. Topics of the session will include the first-principles modelling of metallic nanoparticles reactivity [12], plasmonic structures made by noble-metal nanoparticles [13], and metallic core-shell clusters [14].