ADVANCED ATOMIC-SCALE MODELING FOR NANOPARTICLES FUNCTIONALIZATION

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The functionalization of nanoparticles from molecular building blocks has a wealth of applications ranging from innovative nanomaterials for data storage to biochemical applications and theranostics [1]. Yet, the practical realization of nano-objects assembly relies on the precise understanding of the nature of the fundamental interactions occurring at the surface of a single nano-object and its surrounding environment. In this framework, the present thesis proposes to model at a molecular level the synthesis processes and resulting properties of nanoparticles carrying functional groups for specific material engineering or biomedical applications, depending on the nature of both the nanoparticle and the functional groups. This will be done using the most advanced computational tools in atomic-scale modelling, in synergy with experiments performed at IPCMS [2], aimed at disentangling the factors governing synthesis and functionalization processes.

For the tasks proposed, dynamical simulations involving molecular motion and chemical reactions will be performed within the density functional theory (DFT) framework. For activated processes, enhanced methods for free energy sampling techniques [3,4] will be used. These approaches are available in the computer codes CPMD [5,6] and CP2k [6,7], for which the supervisor of this thesis is co-developer. The same team is also specialized in the accurate choice of the exchange-correlation functionals best adapted to the chemical nature of bonding [8] and is able to tackle with multiscale techniques [4] the relatively large system sizes of the nanoparticle-ligand representative sub-units. The complementary use of the CP2k code is expected to lower the computational costs associated with the largest simulation cells. The PhD candidate will be formed and trained to the use of these codes, an aspect that will contribute to enrich the knowledge of the student in computer simulations, exploitable also in the rest of his/her professional career either in academy or in industry.

This PhD thesis project will be exploit computational resources available at the HPC facility of the University of Strasbourg (EQUIP@MESO) and national centers (IDRIS, CINES, TGCC). Moreover, the experience of our team in the development and use of the most advanced techniques and codes will provide a solid background for the formation of the candidate.

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