Ab-initio-Driven Atomistic Simulations of the Deposition and Aggregation of Nanoscale Metal Particles on Carbon-Based Surfaces at Room Temperature

Ricardo Fernández-Perea[*1], **Luis F. Gómez**[§], **Marti Pi**[¶], **Carlos Cabrillo**[*], **Andrey F. Vilesov**[§ 2], **María Pilar de Lara-Castells**[*3]

[*] Institute of Fundamental Physics, IFF-CSIC, Serrano 123, 28006 Madrid, Spain
[§] Department of Chemistry, University of Southern California, Los Angeles, California, United States
[¶] Facultat de Física, and IN^{2}UB, Universitat de Barcelona, Diagonal 647, 08028 Barcelona, Spain

Synopsis This poster present *ab-initio*-driven atomistic simulations of the deposition and aggregation of nanoscale metal particles on carbon-based surfaces at room temperatures.

The ultra-cold ^{4}He droplet-assisted synthesis and soft deposition of nanoscale metallic particles [1, 2, 3, 4, 5] attracts nowadays strong attention due to both the exciting fundamental physics behind, including quantum vorticity in superfluid ^{4}He droplets [2], and to the applications of deposited metallic and bimetallic core-shell nanoparticles and nanowires [3, 4, 5], such as in catalysis of TiO_2-supported gold nanoparticles [5].

Agreeing well with experimental observations [1], a recent theoretical study demonstrated that the collision of atomic gold immersed in a $^4He_{300}$ droplet onto the $TiO_2(110)$ surface can be characterized as a soft-landing process if the quantum - time-dependent helium density functional-based - description of the helium droplet is applied [6]. In contrast, a classical description of the ^{4}He droplet was unable to explain the soft deposition of atomic species [6]. This poster presents the results of *ab-initio*-driven atomistic simulations [7] addressing the upscaling of the previous study [6] to the aggregation and deposition of a few-nm sized metallic particles (up to 10000 Ag atoms) embedded in large ^{4}He droplets (up to 100000 ^{4}He atoms) and considering two carbon-based surfaces (graphene and amorphous carbon) at room temperature. Our focus will be in comparing simulations with and without inclusion of the ^{4}He droplet dynamics, and in analysing their consistency with recent experimental measurements of Vilesov's group of the deposition and aggregation of silver nanoparticles, onto amorphous carbon at room temperature, using different exposure times.

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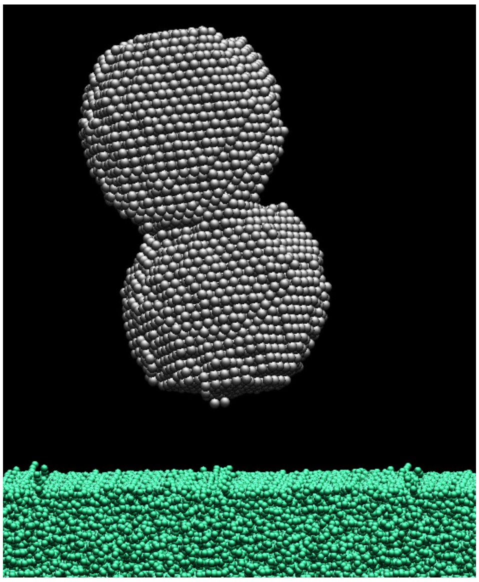

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[1]E-mail: ricardo@langran.iem.csic.es
[2]E-mail: vilesov@usc.edu
[3]E-mail: Pilar.deLara.Castells@csic.es