Solved and Unsolved Problems in Modelling Superfluid Helium Nanodroplet-Mediated Synthesis and Soft-Deposition of a New Generation of Metallic Nanoparticles

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The superfluid helium nanodroplet-mediated synthesis and soft-deposition of metallic nanoparticles [1-6] is attracting the strongest attention nowadays. This is party due to the new fundamental physics revealed, and partly due to their application in producing and depositing onto the target support (in soft-landing conditions), a new generation of stable metallic nano(-photo)catalysts [6], bearing tunable size, shape and composition. We will present both solved and unsolved problems in the theory, modelling and simulation aimed to characterize these exciting molecular processes, including the interphase between the nanoparticle, the fluid helium droplet, and the solid surface. Our first focus will be on ab-initio-based schemes to describe the underlying van-der-Waals dominated interactions, as developed within the framework of the MOLIM COST Action [7-12], including new ab-initio force fields. Our second focus with be on the nuclear dynamics problem: starting with zero-temperature time-dependent density functional theory descriptions of the helium atoms [3], passing through large-scale molecular dynamics simulations of large metallic nanoparticles on corrugated surfaces at finite temperatures [12], and ending with strategies combining both limits.

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