Towards the Helium-mediated Soft-Landing of Embedded Nano-particles on Surfaces: Insights from Ab-initio Simulations

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It is well known that helium nanodroplets can act as cryogenic matrices for high-resolution molecular spectroscopy [1]. Recent experimental measurements [2] have shown that they can also be used as carriers for the "soft-landing" deposition of metal nanoparticles, synthesized inside the droplets, on the surface of different substrates. The development of techniques capable of achieving metal nanoparticles grown, with a narrow size distribution, and deposition in soft-landing conditions is relevant for different surface science applications so that the experimental research on this area has increased considerably during the last two years [3-5]. Ab-initio simulations of these processes hold the potential to reveal the basic mechanistic information and key simplifications. However, they also face many theoretical challenges such as the application of a quantum-mechanical formalism in describing the helium-droplet dynamics [4] or the accurate description of the dispersion-dominated helium-surface interaction [5]. By choosing the TiO_2(110) surface as the substrate, I will present the insights extracted from our first-principle studies.

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