Modeling of the Soft, ^{4}He Droplet-mediated, Deposition of Metallic Nanoparticles: An Intermolecular Interaction Problem

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Abstract

The ultra-cold ^{4}He droplet-assisted synthesis and soft-landing deposition of metallic nanoparticles attracts nowadays strong attention due to both the exciting fundamental physics behind, including quantum vorticity in superfluid ^{4}He droplets [1], and to the applications of the deposited metallic and bimetallic core-shell nanoparticles and nanowires [2-4]. This talk is aimed to present modeling and simulation to deal with this intermolecular interaction problem at the interface between quantum fluid droplets and solid surfaces of different nature [5]. The focus will be in recent ab-initio schemes combining dispersionless density functional, post-Hartree-Fock, and symmetry-adapted perturbation theories to describe He/surface, He/metal, and metal/surface van der Waals-dominated interactions, and the upscaling to nanoscale metallic particles. The application of these schemes to ^{4}He droplets interacting with carbon nanostructures will be also underlined [6].

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