

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

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The ultra-cold ^4He droplet-assisted synthesis and soft-deposition of metallic nanoparticles attracts nowadays strong attention due to both the exciting fundamental physics behind, including quantum vorticity in superfluid ^4He 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 [5–11]. The focus will be in recent ab-initio schemes combining dispersionless density functional [12], incremental post-Hartree-Fock [13], and symmetry-adapted perturbation theories [14] to describe He/surface, He/metal, and metal/surface van der Waals-dominated interactions, as well as the helium density functional approach [15] to account for the time-dependent evolution of the superfluid ^4He droplet motion. The upscaling problem to nanoscale metallic particles will also be discussed. Finally, very recent studies on the intermolecular interaction between ^4He droplets and carbon nanotubes will be underlined [16].

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