AN AB-INITIO-MOTIVATED SCHEME FOR VAN-DER-WAALS ADSORBATE-SURFACE INTERACTIONS: APPLICATION TO TIME-RESOLVED SIMULATIONS OF SOFT, ^{4}HE-DROPLET-ASSISTED, DEPOSITION ON SOLID SURFACES

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The ultra-cold ^{4}He droplet-assisted synthesis and deposition of embedded metal nanoparticles (NPs) on solid surfaces, originally proposed by Vilsesov's group [1], attracts nowadays strong attention [1-5]. This is due to both the exciting fundamental physics revealed via the technique, including earlier traces of quantum vorticity in superfluid ^{4}He droplets [1,5], and the potential applications in nanoscience and nanotechnology [2,3]. For instance, it can be exploited to induce the formation of ultrathin wires of metal NPs [1,5] with special special electro-, magneto-optical, and catalytic properties. To control the metal NPs film formation, it is important to understand the basic mechanism regulating the ^{4}He droplet-mediated deposition of the metal NPs and their subsequent diffusion and aggregation. Of course, this process is much influenced by the specific He-metal, He-surface, and surface-metal interactions so that their accurate descriptions is a prerequisite for realistic first-principles simulations. The first focus of this talk will be on an ab-initio-grounded scheme to van der Waals-dominated adsorbate-surface interactions [6-9,11], with application to the He-surface [7,8,11] and silver-surface systems [9]. Next, we will discuss the dispersionless and dispersion-accounting (time-dependent) density functional and molecular dynamics simulations of ^{4}He droplets at impact with graphene and TiO_2(110) surfaces [8,10,11]. Finally, theoretical evidences for the ^{4}He droplet-assisted-sticking of an embedded metal atom at very low landing energies will be presented [11] (see figure).

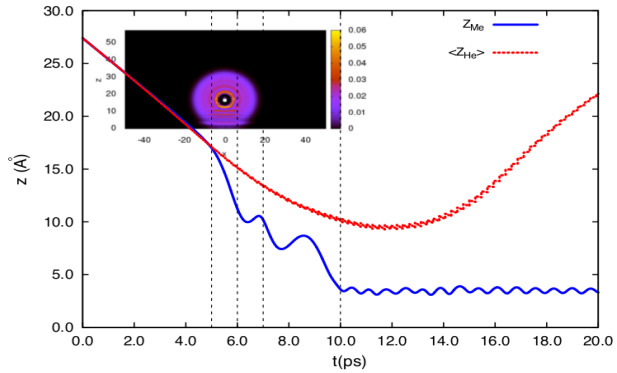

Figure illustrating the ^{4}He-droplet-assisted sticking of a metal atom to a solid surface at very low landing energy. Red and blue lines indicate the position (distance to the surface) of the metal atom and the ^{4}He droplet mass-center as a function of time, respectively.

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