A Combined Periodic Density Functional and Incremental Wave-Function-Based Approach for the Dipersion-Accounting Time-Resolved Dynamics of ^{4}He Nanodroplets on Surfaces: ^{4}He/Graphene

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A general strategy to calculate accurate He-surface interaction potentials is proposed [1]. It extends the dispersionless density functional (dlDF) approach by Pernal et al. [2] to adsorbate-surface interactions by including periodic boundary conditions [1b]. A scheme to parametrize the dispersion interaction is introducced by calculating two- and three-body dispersion terms at CCSD(T) level via the method of increments [3]. The performance of the composite approach is tested on the low-lying selective adsorption states of ^{4}He/graphene [5]. *Second*, its capability to describe dispersionless correlation effects realistically is used to extract dispersion effects in time-dependent density functional simulations on the collision of ^{4}He droplets with graphene [1b]. Dispersion effects play a key role in the fast spreading of the ^{4}He nanodroplet [1b,6], the evaporation-like process of helium atoms, and the formation of solid-like helium structures. These characteristics are expected to be quite general and highly relevant to explain experimental measurements with the newly developed helium droplet mediated deposition technique [7].

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