Helium mediated deposition: Modeling the He−TiO_2(110) interaction potential and application to the collision of a helium droplet from density functional calculations

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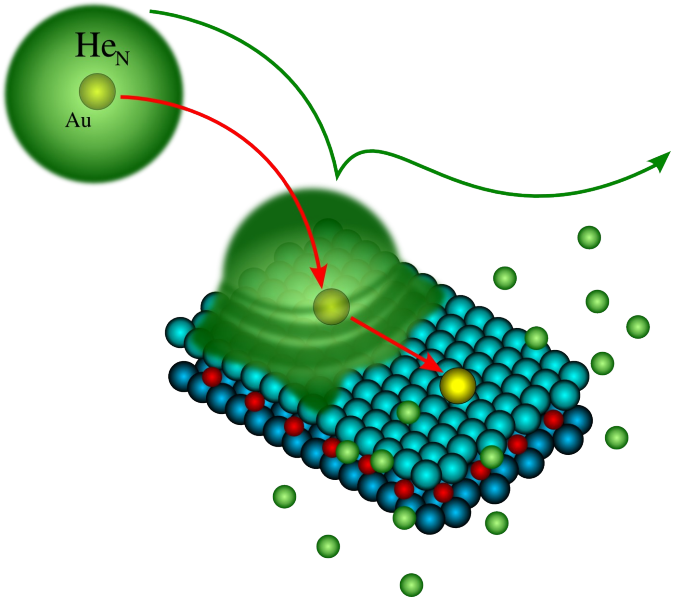
We have studied the interaction of a helium atom with a TiO_2(110) surface as a proto-typical case of physisorption on an transition-metal oxide surface. By using finite cluster and periodic approaches, results show that, once the basis set is specifically tailored to minimize the basis set superposition error, periodic calculations using the PBE (Perdew–Burke–Ernzerhof) functional yield short and medium-range interaction potentials in very reasonable agreement with those obtained using the correlated wave-function-based methods, while small long-range dispersion corrections are necessary to reproduce the correct asymptotic behavior[1]. By using the PBE functional on a numerical grid dense, we built an analytical three-dimensional potential energy surface. Then different model potentials are used to study the dynamics upon collision of a helium droplet with the TiO_2(110) surface at zero temperature within the framework of a time-dependent density-functional approach for the quantum fluid[2] and classical dynamics calculations. At variance with classical dynamics calculations, showing helium droplet splashing out of the surface at impact, the time evolution of the macroscopic helium wave-function predicts that the helium droplet spreads on the rutile surface and leads to the formation of a thin film above the substrate[3]. This work thus provides a basis for simulating helium mediated deposition of metallic clusters embedded within helium nanodroplets.



References

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