Motion of dopants in He-nanodroplets: Challenges and opportunities of a spacial confinement for cluster growth and cold chemistry

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Helium nanodroplets can be considered as spatially confined nano-labs for studies of elementary chemical reactions or the formation of nanoparticles. We combine molecular dynamics simulations with bosonic He-density functional theory to describe the behavior of dopants in their superfuid confinement after pickup. Particle growth will be discussed for the example of the coinage metals Cu, Ag and Au.[1] As a template for studies of He-hindered chemical reactions, we refer to our work on Rb- and Xe-doped small droplets.[2] The fact that molecules with diffuse electron distributions, e.g. alkali metal atoms, prefer to reside on the surface, while others sink into the droplet center, might allow for the arrangement of pre-reactive setups, which could be triggered by photoexcitation. A simple model for electronic excitation of dopants in helium droplets is presented for selected states of the chromium atom.[3,4]

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