Theoretical study of the diffusion of alkali metals on a Cu(111) surface

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We present a theoretical study of the diffusion of Li, Na and K on a Cu(111) surface. Various diffusional paths are identified and characterized in terms of kinetic parameters such as diffusion constants and activation energies. We use a model potential parametrized from DFT calculations to determine adsorption energies, surface corrugation and diffusional behaviors. Two representations of the copper surface (2D and 3D) are used to investigate its effect on the adsorption patterns, diffusion constants and activation energies. An interesting result is that the adsorption pattern for Na and K changes when adding layers of substrate (2D ? 3D) favouring unusual adsorption sites, which is in agreement with recent theoretical evidence.