Survival of hydrogen anions near atomically flat metal surfaces: Band gap confinement and image state recapture effects

ANDREW SCHMITZ, JOHN SHAW, HIMADRI CHAKRABORTY, Northwest Missouri State University, Maryville, MO 64468, UWE THUMM, Kansas State University, Manhattan, KS 66502 — Resonant charge transfer (RCT) between ions and surfaces is a key intermediate step in surface-chemical processes as well as in micro- and nano-fabrications on the surface. The RCT process in the collision of hydrogen anions with metal surfaces is described within a wave packet propagation methodology using Crank-Nicholson algorithm [1]. The ion-survival probability is found to strongly enhance at two different ion velocities perpendicular to the surface. The low velocity enhancement is induced from a dynamical confinement of the ion level inside the band gap, while the high velocity enhancement emerges owing to the recapture from transiently populated image states [2]. These structures are found to be somewhat sensitive to the ion’s distance of closest approach to the surface and the choice of inter-atomic potentials between the ion and the surface atoms. [1] Chakraborty et al., Phys. Rev. A 70, 052903 (2004); [2] Schmitz et al., Phys. Rev. A (submitted).

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