Abstract Submitted for the DAMOP11 Meeting of The American Physical Society

On the role of ion-trajectories on confinement and recapture effects in the survival of anions scattered from metal surfaces¹ ANDREW SCHMITZ, JOHN SHAW, HIMADRI CHAKRABORTY, Northwest Missouri State, Maryville — Resonant charge transfer in ion-surface collisions is a classic tool to explore surface electronic structures. Using the Crank-Nicholson propagation [1] we solve the time-dependent Schroedinger equation to simulate the electronic motion during collisions of H¯with Li(110) and Pd(111) surfaces. It was previously shown that the ion's survival after the collision depends (i) adiabatically (that is at slow ion-speeds normal to the surface) on electrons' confinement in metal band gap and (ii) diabatically on recaptures from image states [2]. We now find that for larger distances of closest approach (DCA) of the ion the image interaction accesses the adiabatic region and dominates the band-gap effect. In a real collision, the flight-trajectory determines the DCA as the metal-lattice repels the ion, resulting in a reduction in ion speed. Hence the trajectory induces a competition between various effects that is found to significantly modify the ion-survival phenomenology.

- [1] Chakraborty et al., Phys. Rev. A **70**, 052903 (2004);
- [2] Schmitz et al., Phys. Rev. A 81, 042901 (2010).

Himadri Chakraborty Northwest Missouri State, Maryville

Date submitted: 31 Jan 2011 Electronic form version 1.4

¹Supported by the NSF and US DoE.