Abstract Submitted for the DAMOP11 Meeting of The American Physical Society

Interactions of hydrogen anions with face-centered-cubic metal surfaces of (110) symmetry¹ JASON SAUERBREI, PETER SABLE, HEE SUK LEE, ANDY SCHMITZ, HIMADRI CHAKRABORTY, Northwest Missouri State, Maryville — Resonant charge transfer in ion-surface collisions determines the survival probability of the ion. The time evolution of the ion's initial electron density provides a microscopic account of the excitation of participating bulk states. We simulate this interaction by solving the time-dependent Schroedinger equation for the H⁻ ion in front of various fcc metal surfaces of (110) symmetry in the same methodology used before for (111) and (100) surfaces [1,2]. The band structures of fcc (110) metals are very unique: The band gap in these metals is formed by the projection of the bulk states along the direction which does not intersect with the bulk Brillouin zone center, allowing for the localization of *two* surface states inside the gap. Using a description of (110) surface [3] our study uncovers important effects of the (110) symmetry on the electrons' motion in general and on the resulting ion survival in particular.

[1] Chakraborty et al., *Phys. Rev.* A **70**, 052903 (2004);

[2] Schmitz et al., Phys. Rev. A 81, 042901 (2010);

[3] Tsirkin et al., Surf. Sc. 604, 804 (2010).

¹Supported by the NSF and US DoE.

Himadri Chakraborty Northwest Missouri State, Maryville

Date submitted: 03 Feb 2011

Electronic form version 1.4