CHARGE TRANSFER BETWEEN H^- ANIONS AND FREE-ELECTRON FLAT AND VICINAL METALLIC SURFACES

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We calculated the ground-state electronic structure of free-electron flat and vicinal metallic surfaces using (i) density functional theory within the Thomas-Fermi-von Weizsäcker model, (ii) a local density approximation for the exchange-correlation energy of the electrons, and (iii) a jellium approximation for the background charge distribution of the positive ionic cores. We included image charge charge effects phenomenologically and derived an effective self-consistent single electron surface potential [1], which we later used to study the electron transfer dynamics between the H^- ion and the surface (Fig. 1).

We evaluated the adiabatic (fixed-ion) shifts and widths of the ion affinity level resonance from the projected density of states of the ion-surface system. We used these shifts and widths to calculate the negative-ion survival probabilities based on a rate equation for a set of classical trajectories for projectiles that are incident with kinetic energies between 50 eV and 1 keV. Our calculations reveal a pronounced left-right scattering asymmetry in the final ion fractions with respect to the orientation of the vicinal surface relative to the incidence direction of the negative ion (Fig. 2). This effect is caused by an enhancement of the electron loss rate on the outgoing part of ion scattering trajectories that approach steps from below [2].

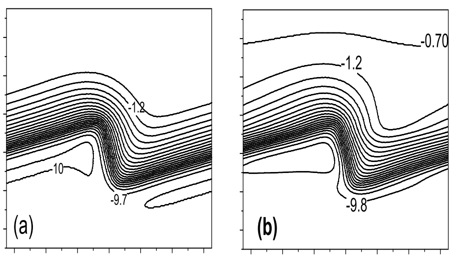

FIG. 1: Contour map of the potential energy of an electron near a vicinal free-electron surface with step height H = 6.82 a.u. and terrace length L = 27.28 a.u. without (a) and with (b) inclusion of image charge effects. The contour line spacing is 0.48 eV. The labels give potential energies (in eV) relative to the vacuum energy level.

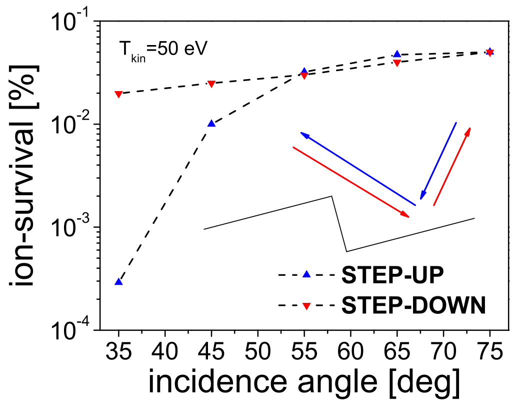

FIG. 2: Ion-survival probability for 50 eV H^- ions after collisions with a free-electron vicinal Cu surface along "step-up" and "step-down" trajectories as a function of the angle of incidence measured with respect to the optical surface plane.

This work was supported by the NSF and the US-DOE.

[1] B. Obreshkov and U. Thumm, Phys. Rev. A **74**, 012901 (2006).
[2] B. Obreshkov and U. Thumm, Surf. Sci. **601**, 622 (2007).