NEUTRALIZATION OF H^- NEAR Si(100) SURFACES

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We calculated the electronic structure of the unreconstructed Si(100) surface within an extended screened Thomas-Fermi pseudopotential method [1]. We derive an effective electronic potential (Fig. 1) from which we obtain single-particle Kohn-Sham orbitals and their energies. Our calculated density of states (DOS) is in good agreement with the observed DOS from photoemission measurements on Si surfaces [2].

We study the charge transfer dynamics between H^- ions with kinetic energies between 50 and 150 eV within the Newns-Anderson model. We calculate the negative ion survival probability $P(H^-) = |S_{aa}|^2 + \sum_{k<k_F} |S_{ak}|^2$ in terms of the survival amplitude S_{aa} of the initial charge state of the ion and amplitudes S_{ak} for capture from the initially occupied Fermi sea of the surface (Fig. 2)

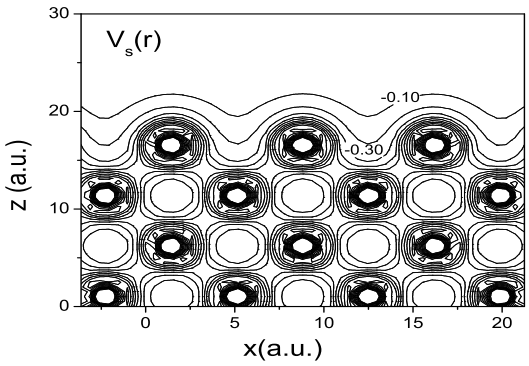

Fig. 1. Contour map of the potential energy of an electron near the Si(100) surface. The contour line spacing is 0.1 a.u. The labels give potential energies relative to the vacuum energy level.

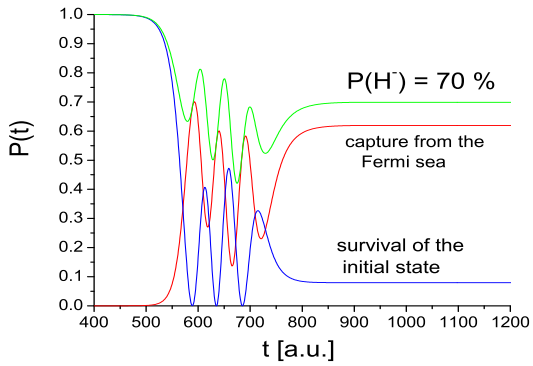

Fig. 2. Survival probability of the incoming H^- ion as a function of time. The ion is incident normal to the surface with a kinetic energy of $E = 150$ eV.

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References

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[2] J. E. Rowe and H. Ibach, PRL **32**, 421 (1974).