High formation of negative ions during collisions between H+ projectiles and a Cu(111) surface.

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Electron transfer between atoms is a fundamental process that has been studied since the beginning of physics and chemistry. Particularly, the charge transfer during collisions between projectile ions and surfaces constitutes one of the bases of the analysis of surfaces [1].

Here, the formation of positive and negative ions in the scattering of protons by a Cu(111) surface is theoretically and experimentally analyzed for a large scattering angle in a backscattering geometric configuration.

The low energy ion scattering (LEIS) technique was used to experimentally determine the ion fractions backscattered after the collision. The collision geometry essentially consisted of a 45º incoming angle and a 90º outgoing angle (both relative to the sample surface); then establishing a 135º scattering angle. The incoming energy was varied from 2 to 8keV.

It was found that the percentage of backscattered ions ranges from 10% to 25%, decreasing with the projectile incoming energy. A peculiarly high yield of negative ions, which always exceeds that of positive ions, was detected for the whole energy range analyzed. The positive ion rate barely depends on the projectile incoming energy.

On the theoretical side, a first principles quantum-mechanical formalism was applied to describe the charge transfer processes involved in the dynamical situation above described [2]. All the physical ingredients involved on the dynamic problem analyzed, such as the crossed terms of the density matrix of the surface solid, the number of surface atoms considered, and the change in the energy level and its width relative to the target surface Fermi level are discriminated and its influence on the partial and final charge states are thoroughly examined. The contrast between theoretical and experimental data allows us to infer how relevant are the different physical ingredients included in the model and the energy range where they play a significant role.

According to our findings: i) the inclusion of the crossed terms of the density matrix introduces a significant change on the projectile energy level and width, ii) the introduction of a large number of surface atoms (up to 37) to describe the solid target are crucial parameters for the calculation. However, the high yield of negative ions is not yet adequately described by the same model that successfully describes the ion faction in the scattering of protons by a HOPG surface [2].

Very approximated preliminary calculations where the excited states of the projectile are also included, indicate that these states could play a key role in the formation of excited states of negative hydrogen ions during the collisional process. The need for the inclusion of these states is, seemingly, strongly linked to a less efficient neutralization to the ground state due to the proximity of the ionization energy level of the projectile to the bottom of the surface valence band.

References

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