

Universidade de São Paulo
Instituto de Física de São Carlos

XIV Semana Integrada do Instituto de
Física de São Carlos

Livro de Resumos da Pós-Graduação

São Carlos
2024

Ficha catalográfica elaborada pelo Serviço de Informação do IFSC

Semana Integrada do Instituto de Física de São Carlos
(13: 21-25 ago.: 2023: São Carlos, SP.)

Livro de resumos da XIII Semana Integrada do Instituto de
Física de São Carlos – Universidade de São Paulo / Organizado
por Adonai Hilário da Silva [et al.]. São Carlos: IFSC, 2023.
358p.

Texto em português.

1.Física. I. Silva, Adonai Hilário da, org. II. Título.

ISSN: 2965-7679

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Non-adiabatic contributions to the sticking coefficient for atoms impinging on metallic surfaces

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We are interested in the adhesion rate that occurs from the collision process between an atom or molecule and a surface. This adsorption mechanism is of great importance in the fields of Physics and Chemistry, explaining phenomena such as catalysis and corrosion. Qualitatively, the problem can be described by a neutral atom initially approaching a metallic surface. The overlap between the orbitals of this atom and those of the surface increases, allowing charge transfer. When an electron is transferred, the atom acquires an electric charge, and consequently, an image charge potential appears, accelerating the particle toward the surface. In the subsequent collision, the generation of phonons and electron-hole pairs in the metal robs energy from the incident atom, which may become trapped in the attractive potential. Therefore, there is a probability that this particle will be adsorbed by the surface. The theoretical challenge is to calculate this probability, known as the Stiking coefficient, S . The Born-Oppenheimer approximation, traditionally used to separate the nuclear part from the electronic wavefunction, is not capable of explaining this phenomenon. Moreover, we cannot use adiabatic approximations since it is precisely the non-adiabatic effects that allow the atom's energy loss. Therefore, a full calculation employing a precise numerical treatment of the time-dependent wavefunction $\Psi(z, t)$ is necessary. Simplified, the procedure to find the adhesion coefficient S is based on calculating the spectrum of electronic energies using the Numerical Renormalization Group (NRG) method (1) for each value of the distance z . In the initial state, the particle is far from the surface, and its wavefunction is the product of the initial electronic state and a Gaussian centered at an initial position, which describes the nuclear part. The Crank-Nicolson method (2) is used to calculate the time evolution of the wavefunction until, after the collision, the function splits into one part localized near the surface and another moving away from it. The spatial integral of the square modulus of the first part determines the Sticking coefficient S . In our findings for H-Cu surface collisions, if the H atom moves slowly close to the Cu surface, the Hamiltonian changes gradually, and only small energy particle-hole excitations will be significant. Since there is no dissipative term in the Hamiltonian, the atom will merely accelerate and collide with the surface, rebound, and lose the kinetic energy gained from the image-charge potential. No interesting physics emerges from this reversible collision, and the sticking coefficient approaches zero. Conversely, if the initial kinetic energy is high, the system does not have enough time to hybridize; the resulting sticking coefficients are equally small. Only at intermediate energy scales, around $K_0 \sim 0.3$ eV, does the probability of binding to the surface become significant $S \sim 30\%$.

Palavras-chave: Sticking coefficient; Atomic-surface collision; Non-adiabatic behavior

Agência de fomento: CAPES (88887.495890/2020-00)

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