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Hydrogen dissociation on metal surfaces

Wijzenbroek, M.

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Hydrogen dissociation on metal surfaces

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door

Mark Wijzenbroek
geboren te Vlaardingen in 1988

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Promotor: prof. dr. G. J. Kroes
Overige leden: prof. dr. J. Brouwer
prof. dr. M. T. M. Koper
prof. dr. J. G. E. M. Fraaije
prof. dr. A. Groß (Universität Ulm)
dr. C. Díaz (Universidad Autónoma de Madrid)
dr. L. B. F. Juurlink
dr. J. Meyer

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List of acronyms

AIMD	<i>ab initio</i> molecular dynamics.
BOSS	Born–Oppenheimer static surface.
BtH	bridge-to-hollow.
CRP	corrugation reducing procedure.
CT	classical trajectory.
DFT	density functional theory.
DVR	discrete variable representation.
DW	Debye–Waller.
FBR	finite base representation.
FCC	face-centered cubic.
FFT	fast Fourier transform.
GGA	generalized gradient approximation.
HCP	hexagonal close packed.
HEG	homogeneous electron gas.
LDA	local density approximation.
meta-GGA	meta-generalized gradient approximation.
ML	monolayer.
MSO	modified surface oscillator.

NEB	nudged elastic band.
PAW	projector augmented wave.
PES	potential energy surface.
QCT	quasi-classical trajectory.
QD	quantum dynamics.
RMSE	root mean square error.
SCM	static corrugation model.
SM	surface mass.
SO	surface oscillator.
SRP	specific reaction parameter.
TD-DFT	time-dependent density functional theory.
TDWP	time-dependent wave packet.
TOF	time-of-flight.
TtB	top-to-bridge.
USPP	ultrasoft pseudopotential.
XC	exchange–correlation.
ZPE	zero-point energy.

List of symbols

Coordinates of a diatomic molecule

U	Lateral position of the center of mass of a diatomic molecule with respect to the surface (skewed coordinates).
V	Lateral position of the center of mass of a diatomic molecule with respect to the surface (skewed coordinates).
X	Lateral position of the center of mass of a diatomic molecule with respect to the surface (Cartesian coordinates).
Y	Lateral position of the center of mass of a diatomic molecule with respect to the surface (Cartesian coordinates).
Z	Distance of the center of mass of a diatomic molecule to the surface.
φ	Azimuthal angle of a diatomic molecule.
ϑ	Polar angle of a diatomic molecule.
\vec{r}	Collection of $U, V, Z, r, \vartheta, \varphi$.
r	Bond length of a diatomic molecule.

Coordinates of an atom

$\vec{\rho}$	Collection of u, v, z .
u	Lateral position of an atom with respect to the surface (skewed coordinates).

v	Lateral position of an atom with respect to the surface (skewed coordinates).
z	Distance of an atom to the surface.

Corrugation reducing procedure

I^{3D}	Three-dimensional interpolation function.
I^{6D}	Six-dimensional interpolation function.
V^{1D}	Repulsive pair potential used for the calculation of I^{3D} .
V^{3D}	Three-dimensional potential energy surface.
V^{6D}	Six-dimensional potential energy surface.

Density functional theory

E_{XC}	Exchange–correlation functional.
V_H	Hartree potential.
V_{KS}	Kohn–Sham potential.
V_{XC}	Exchange–correlation potential.
V_{ext}	External potential.
ϵ_C	Correlation energy per particle.
ϵ_{XC}	Exchange–correlation energy per particle.
ϵ_X	Exchange energy per particle.
n	Electron density.

Geometry of the surface

\vec{q}_{id}	Collection of all surface degrees of freedom for an ideal surface.
\vec{q}	Collection of all surface degrees of freedom.
d_{a-b}	Distance between layers a and b .

Initial conditions

E_{\perp}	Perpendicular translational energy of a molecule.
E_{rot}	Rotational energy of a molecule.
E_{trans}	Translational energy of a molecule.
E_{vib}	Vibrational energy of a molecule.

E_{\parallel}	Parallel translational energy of a molecule.
L	Magnitude of the angular momentum vector.
T_n	Nozzle temperature.
T_{rot}	Rotational temperature.
T_s	Surface temperature.
α	Width of the velocity distribution of a molecular beam.
φ_i	Angle of incidence of the molecule (angle between the projection of the velocity vector on the (U, V) plane and the U axis).
ϑ_L	Angle between the angular momentum vector and the surface normal.
ϑ_i	Angle of incidence of the molecule (angle between the velocity vector and the surface normal).
v_0	Stream velocity of a molecular beam.
v_i	Incident velocity of a molecule.

Observables

$A_0^{(2)}$	Rotational quadrupole alignment parameter.
P_{deg}	Degeneracy averaged initial state-resolved reaction probability.
P_{scat}	State-to-state scattering probability.
P_r	Fully initial state-resolved reaction probability.
χ_ν	Vibrational efficacy.

Physical constants

k_B	Boltzmann constant.
\hbar	Reduced Planck constant.

Properties of the potential

E_b	Height of a barrier.
Z_b	Z coordinate at a barrier.
ξ	Energetic corrugation.
r_b	r coordinate at a barrier.

Quantum numbers

J'	Final rotational quantum number of a diatomic molecule.
J	Initial rotational quantum number of a diatomic molecule.
ν'	Final vibrational quantum number of a diatomic molecule.
ν	Initial vibrational quantum number of a diatomic molecule.
m'_J	Final magnetic rotational quantum number of a diatomic molecule.
m_J	Initial magnetic rotational quantum number of a diatomic molecule.
m	A diffraction quantum number of a diatomic molecule interacting with a surface.
n	A diffraction quantum number of a diatomic molecule interacting with a surface.

Reaction probability curve parameters

A	Saturation value of a reaction probability curve.
E_0	Dynamical barrier height.
W	Width of a reaction probability curve.

Static corrugation model

V_{coup}	Coupling potential.
V_{strain}	Strain potential.