Hydrogen dissociation on metal surfaces

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PROEFSCHRIFT

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Contents

List of acronyms

AIMD	*ab initio* 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, ϑ, φ.
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 surfaces 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.