Getting the electrons right for O2-on-metal systems

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List of abbreviations, acronyms, and symbols

A list of abbreviations, acronyms, and symbols commonly used in the thesis:

AES: *Auger electron spectroscopy*
AIMD: *Ab initio molecular dynamics*

BOA: *Born-Oppenheimer approximation*
BOMD: *Born-Oppenheimer molecular dynamics*
BOSS: *Born-Oppenheimer static surface*
BuSA: *Burlisch–Stoer algorithm*

CRP: *Corrugation reducing procedure*
COM: *Centre-of-mass*

DC: *Dissociative chemisorption*
DCM: *Dynamic corrugation model*
DF: *Density functional*
DFT: *Density functional theory*
DOF: *Degrees of freedom*

EA: *Electron affinity*
E_{av}: *Average energy of the molecular beam*
E_{CT}: *Charge transfer energy;* ϕ *-* EA
ECW: *Embedded correlated wavefunction*
E^{HF}: *Hartree Fock exchange energy*
Ehp: *Electron-hole-pair*
E_i: *Incidence energy*
$E_i^{\perp}$: *Normal incidence energy*
E_{kin}: *Kinetic energy*
E_{ro}: *Rotational energy*
E_{rovib}: *Rovibrational energy*
E_s: *Stream energy of the molecular beam*
E_{vib}: *Vibrational energy*
E_{XC}: *Exchange-correlation energy*

FCC: *Face-centred cubic*
FFT: *Fast-Fourier transform*

GGA: *Generalised gradient approximation*
GLO: *Generalised Langevin oscillator*

HDNN: *High dimensional neural-network*
HK: *Hohenberg-Kohn*
HF: *Hartree-Fock*
HREELS: *High-resolution electron energy loss spectroscopy*

K&W: *King & Wells*
KS: *Kohn-Sham*

LDA: *Local density approximation*
LEED: *Low energy electron diffraction*

MD: *Molecular dynamics*
mGGA: *Meta-generalised gradient approximation*

N: *Normal orientation; $\theta = 0°$*
NSCF: Non-*self-consistent field*
NES: *Normal energy scaling*

P: *Parallel orientation; $\theta = 90°$*
PAW: *Projector augmented wave*
PBC: *Periodic Boundary Conditions*
P_E: *Event probability*
PES: *Potential energy surface*
P_r: *Reaction probability*
P_r^D: *Direct reaction probability*
P_r^I: *Indirect reaction probability*
P_r^T: *Total reaction probability*
P_s: *Scattering probability*
P_t: *Trapping probability*

QCT: *Quasi-classical trajectory*
QD: *Quantum dynamics*

Ref.: *Reference*
RMSE: *Root mean squared error*

S_0: *Sticking probability; $1 - P_s$*
SCF: *Self-consistent field*
SCM: *Static corrugation model*
S_H: *S_0 of helicoptering molecules*
S_P: *S_0 of perpendicular molecules*

T: *Tilted orientation; $\theta = 45°$*
T_N: *Nozzle temperature*
TOF: *Time-of-flight*
T_s: *Surface temperature*
TS: *Transitions state*

VASP: *Vienna Ab Initio Simulation Package*
V_{av}: *Average velocity of the molecular beam*
VdW: *Van der Waals*
V_s: *Stream velocity of the molecular beam*

XC: *Exchange-correlation*
XPS: *X-ray photon spectroscopy*

ZPE: *Zero-point energy*

ΔE_S: *Distribution width of the energy of the molecular beam*
ΔV_S: *Distribution width of the velocity of the molecular beam*
Θ: *Incidence angle of the molecular beam*
ϕ: *Work function*