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# 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;* $\phi$ *-* $EA$
**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*

$\Delta E_S$: *Distribution width of the energy of the molecular beam*
$\Delta V_S$: *Distribution width of the velocity of the molecular beam*
**Θ**: *Incidence angle of the molecular beam*
**ϕ**: *Work function*