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# List of abbreviations and symbols

BSSE	Basis set superposition error
DFT	Density functional Theory
DOS (PDOS)	Density of states or Projected density of states
EELS (HREELS or VEELS)	Electron energy loss spectroscopy ( High resolution electron energy loss spectroscopy or vibrational energy loss spectroscopy)
$E_{\text{ads}}$	Adsorption energy
$E_{\text{C}_x\text{H}_y/\text{surface}}$	Energy of the system adsorbate-surface
$E_{\text{C}_x\text{H}_y(\text{g})}$	Energy of the hydrocarbon in the gas phase
$E_{\text{surface}}$	Energy of the surface
$E_{\text{reac}}$	Reaction energy
$E_{\text{TS}}$	Energy of the transition state
GGA	Generalised gradient approximation
H-L	HOMO (highest occupied molecular orbital)–LUMO (lowest unoccupied molecular orbital)
$I_i$	Intensity
IR	Infrared
IRIAN	
LDA	Local density approximation
LEED (LEED- IV)	Low energy electron diffraction (Low energy electron diffraction-Intensity voltage)
MEP	Minimum energy path
MSSR	Metal surface selection rules
NEB	Nudged elastic band
PAW	Projector augmented wave
PhD	Photoelectron diffraction
PW91	Perdew-Wang 91
RAIRS	Reflection absorption infrared spectroscopy
RECP	Relativistic effective core potentials
TDS	Thermal desorption spectroscopy
TS	Transition state
UHV	Ultra high vacuum
US-PP	Ultra soft pseudo potentials
VASP	Vienna ab initio simulation package
ZPE	Zero point energy
$\nu_i$	Experimental frequency
$\omega_i$	Harmonic calculated frequency
$\theta$	Coverage