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List of abbreviations

AA	Ascorbic Acid
ADMM	Auxiliary Density Matrix Method
AIMD	*Ab Initio* Molecular Dynamics
B3LYP	XC-functional approximation by Becke, Lee, Yang and Parr
bda^{2-}	2,2′-bipyridine-6,6′-dicarboxylic acid
BO	Born-Oppenheimer
bpy	2,2'-bipyridine
CB	Conduction Band
CBM	Conduction Band Minimum
COSMO	COnductor like Screening MOdel
CSVR	Canonical Sampling Through Velocity Rescaling
CT	Charge Transfer
CV	Cyclic Voltammetry
cy	p-cymene
D-A	Donor-Acceptor
DFT	Density Functional Theory
DMF	Dimethylformamide
DOS	Density of States
DS-PEC	Dye-Sensitized Photoelectrochemical Cell
DVP	Differential Pulse Voltammetry
DZP	Double-ζ Polarized
ED	Electron Donor
EH	Extended Hückel
EPR	Electronic Paramagnetic Resonance
ET	Electron Transfer
FCDW	Franck-Condon-Debye-Waller
FES	Free Energy Surface
FSSH	Fewest Switches Surface Hopping
GGA	Generalized Gradient Approximation
GSB	Ground State Bleach
HAT	Hydrogen Atom Transfer
hBN	Hexagonal Boron Nitride
HEC	Hydrogen Evolution Catalyst
HER	Hydrogen Evolution Reaction
HFX	Hartree-Fock exchange
HOMO	Highest Occupied Molecular Orbital
HSE06	XC-functional approximation by Hyed, Scuseria and Ernzerhof
I2M	Interaction of two Metal centers

IRC	Internal Reaction Coordinate
LDA	Local Density Approximation
LSV	Linear Sweep Voltammetry
LUMO	Lowest Unoccupied Molecular Orbital
MD	Molecular Dynamics
NDI	2,6-diethoxy-1,4,5,8-diimidenapthalene
NHE	Normal Hydrogen Electrode
NMR	Nuclear Magnetic Resonance
NTO	Natural Transition Orbital
OER	Oxygen Evolution Reaction
OPBE	XC-functional approximation which combines Handy's Optimized exchange with PBE correlation
OT	Orbital Transformation
P1	4-(bis-4-(5-(2,2-dicyano-vinyl)-thiophene-2-yl)-phenyl-amino)-benzoic acid
PBC	Periodic Boundary Conditions
PBE	XC-functional approximation by Perdew, Burke and Ernzerhof
PCET	Proton-Coupled Electron Transfer
PDOS	Projected Density of States
PEG	Polyethylene Glycol
PEM	Proton Exchange Membrane
pic	4-picoline
PS	Photosensitizer
PV	Photovoltaic
PW	Plane Wave
RDS	Rate-Determining Step
SAS	Species Associated Spectra
SE	Stimulated Emission
SF-TDDFT	Spin-Flip Time-Dependent Density Functional Theory
SHE	Standard Hydrogen Electrode
SP	Survival Probability
TA	Transient Absorption Spectroscopy
TBAPF6	tetrabutylammonium hexafluorophosphate
TCEP	tris(2-carboxyethyl)phosphine hydrochloride
TDDFT	Time-Dependent Density Functional Theory
TOF	Turnover Frequency
TON	Turnover Number
TS	Transition State
TZP	Triple-ζ Polarized
UEG	Uniform Electron Gas
VB	Valence Band
VBM	Valence Band Maximum

VDOS	Vibrational Density of States
WNA	Water Nucleophilic Attack
WOC	Water Oxidation Catalyst
XC	Exchange-Correlation
ZORA	Zeroth Order Regular Approximation
ZPL	Zero Phonon Line