Photoinduced processes in dye-sensitized photoanodes under the spotlight: a multiscale in silico investigation

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Photoinduced Processes in Dye-Sensitized Photoanodes under the Spotlight: A Multiscale *in Silico* Investigation

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To my parents and Anna

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List of Abbreviations

ACC	Acceptor
ADF	Amsterdam Density Functional (*program*)
ADP	Adenosine Diphosphate
AIMD	Ab Initio Molecular Dynamics
ALDA	Adiabatic Linear Density Approximation (*XC kernel*)
AMS	Amsterdam Modelling Suite (program)
AO	Atomic Orbital
ATP	Adenosine Triphosphate
Ben-NDI	Benzoic acid-based core extended Naphthalene Diimide dye
BJ	Becke-Johnson (*type of damping function for D3 dispersion corrections*)
BLYP	Becke, Lee-Yang-Parr (*XC functional*)
BOA	Born-Oppenheimer Approximation
BOMD	Born-Oppenheimer Molecular Dynamics
B3LYP	Becke, 3-parameter, Lee-Yang-Parr (*XC functional*)
CAM-B3LYP	Coulomb Attenuating Method – B3LYP (*XC functional*)
Cat-NDI	Catechol-based core extended Naphthalene Diimide dye
CB	Conduction Band
COSMO	Conductor-like Screening Model (*implicit solvent model*)
CT	Charge Transfer
CTD	Charge Transfer Dynamics
CV	Cyclic Voltammetry
DCM	Dichloromethane
DFT	Density Functional Theory
DFT-D3	DFT with D3 dispersion corrections
DFTB	Density Functional based Tight Binding
DNA	Deoxyribonucleic Acid (chap 3)
DON	Donor
DOS	Density Of States
DPA	Diphenylamine
DS-PEC	Dye Sensitized Photoelectrochemical Cell
DSSC	Dye Sensitized Solar Cell
DZP	Double Zeta with one Polarization function (*basis set*)
D3	*Type of Dispersion corrections*

EDG	Electron Donating Group
EH	Extended Hückel
ET	Electron Transfer
ETD	Electron Transfer Dynamics
FC	Franck Condon
FLU	Fluorene
FLUMe	Methylated Fluorene
FT	Fourier Transform
GBSA	Generalized Born accessible Surface Area model (*implicit solvent model*)
GFN-xTB	Geometry, Frequency, Non-covalent Interactions Extended Tight Binding
GGA	Generalized Gradient Approximation
HEC	Hydrogen Evolution Catalyst
HEG	Homogeneous Electron Gas
HOMO	Highest Occupied Molecular Orbital
Hyd-NDI	Hydroxamic acid-based core extended Naphthalene Diimide dye
ISC	Intersystem Crossing
I2M	Interaction of two Metal oxo species
LC	Long-range Corrected
LDA	Local Density Approximation
LR-TDDFT	Linear Response Time Dependent Density Functional Theory
LUMO	Lowest Unoccupied Molecular Orbital
MCTDH	Multi Configurational Time Dependent Hartree
MD	Molecular Dynamics
MO	Molecular Orbital
$NADP^+$/NADPH	Nicotinamide Adenine Dinucleotide Phosphate
NAMD	Non Adiabatic Molecular Dynamics
NCAP	Nonadiabatic Conversion via Adiabatic Passage
NDI	Naphthalene Diimide
NHE	Normal Hydrogen Electrode
NMR	Nuclear Magnetic Resonance
OEC	Oxygen Evolving Complex
OPBE	Optimized exchange Perdew-Burke-Ernzerhof (*XC functional*)
PBE	Perdew-Burke-Ernzerhof (*XC functional*)

PCET	Proton Coupled Electron Transfer
PDOS	Partial Density Of States
PEM	Proton Exchange Membrane
PMI	Perylene-Monoimide
PMIMe	Methylated PMI
PSI	Photosystem I
PSII	Photosystem II
rev-DOD-BLYP	Revised, Dispersion corrected, constrained, Double hybrid-BLYP (*XC functional*)
rev-DOD-PBE	Revised, Dispersion corrected, constrained, Double hybrid-PBE (*XC functional*)
rev-DOD-PBEP86	Revised, Dispersion corrected, constrained, Double hybrid-PBEP86 (*XC functional*)
ROC	Radical Oxo Coupling
SCC-DFTB	Self-Consistent Charge Density Functional based Tight Binding
SCM	Software for Chemistry and Materials (*company*)
SPH	Single Point Hessian
STO	Slater Type Orbital
TD-DFT	Time Dependent Density Functional Theory
TEMPO	2,2,6,6-Tetramethylpiperidine 1-oxyl
TPA	Triphenylamine
TPAMe	Methylated TPA
TZP	Triple Zeta with one Polarization function (*basis set*)
VB	Valence Band
VDOS	Vibrational Density Of States
WNA	Water Nucleophilic Attack
WOC	Water Oxidation Catalyst
XC	Exchange Correlation
ZORA	Zero-Order Regular Approximation (*model for relativistic effects*)
ZPE	Zero Point Energy
ΔSCF	Delta Self Consistent Field (*method to estimate ionization potential*)