Taking control of charge transfer : strategic design for solar cells

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Taking Control of Charge Transfer:

Strategic Design for Solar Cells

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Cover designed by Adriano Monti

To my parents, my family, and my grandparents.

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List of Abbreviations

ADF	:	Amsterdam Density Functional
AO	:	Atomic Orbital
BO	:	Born-Oppenheimer
CB	:	Conduction Band
CDFT	:	Constrained Density Functional Theory
COSMO	:	Continuum Solvation Model
CPMD	:	Carr-Parrinello Molecular Dynamics
CS	:	Charge Separated State
CTI	:	Charge Transfer Integrals
D-A	:	Donor-Acceptor
D-An-A	:	Donor-Antenna-Acceptor
DCM	:	Dichloromethane
DFT	:	Density Functional Theory
DOS	:	Density of States
DS-PEC	:	Dye-Sensitized Photoelectrochemical Cells
DSSC	:	Dye-Sensitized Solar Cell
EA	:	Electron Acceptor
ED	:	Electron Donor
EHT		Extended Hückel Theory
EQD	:	Electron Quantum Dynamics
ET	:	Electron Transfer
FMO	:	Frontier Molecular Orbital
FNR	:	Ferredoxin-$NADP^+$ Reductase
GGA	:	Generalized Gradient Approximation
HF	:	Hartree-Fock
HK	:	Hohenberg-Kohn
HEC	:	Hydrogen Evolving Catalyst
HOMO	:	Highest Occupied Molecular Orbital
LC	:	Long-range Corrected
LDA	:	Local Density Approximation

LUMO	:	Lowest Unoccupied Molecular Orbital
MO	:	Molecular Orbital
NDI_1	:	2,6-diethoxy-1,4,5,8-diimidenaphthalene
NDI_2	:	2,6-dicarbonitrile-1,4,5,8-diimidenaphthalene
OEC	:	Oxygen Evolving Center
PBC	:	Periodic Boundary Condition
PCET	:	Proton-Coupled Electron Transfer
PEM	:	Proton Exchange Membrane
PES	:	Potential Energy Surface
Ph	:	Phenyl Ring
Ph	:	Phenyl bridge
PSII	:	Photosystem II
PTZ	:	10,10a-dihydro-4aH-phenothiazine
PW	:	Plane Waves
SP	:	Survival Probability
STO	:	Slater-type orbitals
TD-DFT	:	Time-dependent density functional theory
TDKS	:	Time-dependent Kohn Sham
VB	:	Valence Band
WOC	:	Water Oxidation Catalyst
xc	:	Exchange-Correlation