Coherent Dynamics in Solar Energy Transduction

PROEFSCHRIFT

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Symbols

$\boldsymbol{a}, \boldsymbol{A}$	*vector $\vec{a}, \vec{A}$ (bold)*
a_{ij}	*density matrix element*
$a(t)$	*acceleration*
$c_i(t)$	*time-dependent coefficient*
$\chi(\boldsymbol{R}(t))$	*nuclear wavefunction*
$d_{ij}(\boldsymbol{r}, \boldsymbol{R}(t))$	*nonadiabatic coupling*
ϵ_i	*orbital energy*
ε_i	*photon energy*
E	*energy*
$E_0(\boldsymbol{R}(t))$	*ground state energy*
$E_i(\boldsymbol{R}(t))$	*excited state energy*
$\hat{\mathcal{H}}(\boldsymbol{r}, \boldsymbol{R}(t))$	*Hamiltonian operator*
$\hat{\mathcal{H}}_e(\boldsymbol{r}, \boldsymbol{R}(t))$	*electronic Hamiltonian*
$\hat{\mathcal{H}}_{ij}(\boldsymbol{r}, \boldsymbol{R}(t))$	*Hamiltonian matrix element*
f_i	*oscillator strength*
F	*force*
γ_c	*bath correlation time*
$\Gamma(t)$	*density matrix*
ΔG	*free energy difference*
λ	*reorganization energy*
$\hat{\mu}$	*dipole moment operator*
M	*mass*
N	*number of electrons*
∇_i	*differential operator*
O	*observable*
$\phi(\boldsymbol{r})$	*molecular orbital*
$\varphi(\boldsymbol{r}, t)$	*time-dependent molecular orbital*
$\psi(\boldsymbol{r}; \boldsymbol{R}(t))$	*electronic wavefunction*
$\Psi(\boldsymbol{r}, \boldsymbol{R}(t))$	*electron-nuclear wavefunction*
$\Psi(\boldsymbol{r}, \boldsymbol{R}, t)$	*total time-dependent wavefunction*
$PSD(\boldsymbol{r}, t)$	*photoinduced spin density*
ρ	*electron density*
ρ_0	*ground state electron density*

$\rho^{\alpha,\beta}$	*spin polarized electron density*
$\boldsymbol{r}$	*electronic coordinate*
$\boldsymbol{R}$	*nuclear coordinate*
$\boldsymbol{R}(t)$	*nuclear trajectory*
$\boldsymbol{R}'(t)$	*specific nuclear motion*
t	*time*
Δt	*timestep*
$\hat{T}$	*kinetic energy operator*
v	*single particle potential*
V	*potential energy*
V_{el-el}	*electron-electron potential*
V_{el-n}	*electron-nucleus potential*
V_{n-n}	*nucleus-nucleus potential*
$v(t)$	*velocity*
$\hat{W}$	*electronic population operator*
$x(t)$	*position*
Z_I	*nuclear charge*

Abbreviations

ADF	*Amsterdam Density Functional*
AIMD	*Ab Initio Molecular Dynamics*
BiP	*Benzimidazolephenol*
BLYP	*Becke Lee Yang Parr*
bRC	*Bacterial Reaction Center*
CCSD	*Coupled Cluster Singles and Doubles*
CDFT	*Constrained Density Functional Theory*
COSMO	*Conductor-Like Screening Model*
CPMD	*Car-Parrinello Molecular Dynamics*
CT	*Charge Transfer*
DCACP	*Dispersion Corrected Atom Centered Pseudopotentials*
DFT	*Density Functional Theory*
ENDOR	*Electron Nuclear Double Resonance*
EOM	*Equations of Motion*
EPR	*Electron Paramagnetic Resonance*
ET	*Electron Transfer*
GGA	*Generalized Gradient Approximation*
HF	*Hartree-Fock*
HOMO	*Highest Occupied Molecular Orbital*
HSD	*Hole Spin Density*
LDA	*Local Density Approximation*
LUMO	*Lowest Unoccupied Molecular Orbital*
MM	*Molecular Mechanics*
MPI	*Message Passing Interface*
NDI	*Napthalene Diimide*
NMR	*Nuclear Magnetic Resonance*
OCTOPUS	*Open-Source Software for Real-Time TDDFT*
OEC	*Oxygen Evolving Complex*
PCET	*Proton-Coupled Electron Transfer*
PDB	*Protein Data Bank*
PES	*Potential Energy Surface*
PSII	*Photosystem II*
PSD	*Photoinduced Spin Density*

QM	*Quantum Mechanics*
RC	*Reaction Center*
RMSD	*Root Mean Square Displacement*
ROKS	*Restricted Open-Shell Kohn Sham*
TDDFT	*Time-Dependent Density Functional Theory*
TZP	*Triple Zeta Polarized Basis Set*
VDOS	*Vibrational Density of States*