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Coherent Dynamics in Solar Energy Transduction

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Symbols

\mathbf{a}, \mathbf{A}	vector \vec{a}, \vec{A} (bold)
a_{ij}	density matrix element
$a(t)$	acceleration
$c_i(t)$	time-dependent coefficient
$\chi(\mathbf{R}(t))$	nuclear wavefunction
$d_{ij}(\mathbf{r}, \mathbf{R}(t))$	nonadiabatic coupling
ϵ_i	orbital energy
ε_i	photon energy
E	energy
$E_0(\mathbf{R}(t))$	ground state energy
$E_i(\mathbf{R}(t))$	excited state energy
$\hat{\mathcal{H}}(\mathbf{r}, \mathbf{R}(t))$	Hamiltonian operator
$\hat{\mathcal{H}}_e(\mathbf{r}, \mathbf{R}(t))$	electronic Hamiltonian
$\hat{\mathcal{H}}_{ij}(\mathbf{r}, \mathbf{R}(t))$	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
$\phi(\mathbf{r})$	molecular orbital
$\varphi(\mathbf{r}, t)$	time-dependent molecular orbital
$\psi(\mathbf{r}; \mathbf{R}(t))$	electronic wavefunction
$\Psi(\mathbf{r}, \mathbf{R}(t))$	electron-nuclear wavefunction
$\Psi(\mathbf{r}, \mathbf{R}, t)$	total time-dependent wavefunction
$PSD(\mathbf{r}, t)$	photoinduced spin density
ρ	electron density
ρ_0	ground state electron density

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

Abbreviations

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

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