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|---|---|
| **ACN** | acetonitrile |
| **ACQ** | aggregation caused quenching |
| **ADC** | algebraic diagrammatic construction |
| **AEEE** | aggregation enhanced excimer emission |
| **AIE** | aggregation induced emission |
| **AIEE** | aggregation induced enhanced emission |
| **AIPE** | aggregation induced phosphorescent emission |
| **bpy** | bipyridine |
| **CASPT2** | complete active space with second-order perturbation theory |
| **CASSCF** | complete active space self-consistent field |
| **CBE** | conduction band edge |
| **CI** | conical intersection |
| **CIEE** | crystallization induced emission enhancement |
| **CIP** | crystallization induced phosphorescence |
| **CIS** | configuration interaction singles |
| **CMFs** | color matching functions |
| **CT** | charge transfer |
| **DCM** | dichloromethane |
| **DFT** | density functional theory |
| **DMSO** | dimethylsulfoxide |
| **DMTPS** | dimethyl tetraphenylsilole |
| **DPDBF** | diphenyldibenzofulvene |
| **DSSC** | dye-sensitized solar cell |
| **ECP** | effective core potential |
| **EML** | emission layer |
| **EOM-CC** | equation-of-motion coupled cluster |
| **EPESS** | enhanced phosphorescence emission in the solid state |
| **ESIPT** | excited state intramolecular proton transfer |
| **ESOP** | excited state oxidation potential |
| **ETL** | electron transport layer |
| **FC** | Franck-Condon |
| **FTO** | fluorine-doped tin oxide |
| **GSOP** | ground state oxidation potential |
| **HF** | Hartree-Fock |

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|---|---|
| **HOMO** | highest occupied molecular orbital |
| **HPS** | hexaphenylsilole |
| **HR** | Huang-Rhys |
| **HTL** | hole transport layer |
| **IC** | internal conversion |
| **ILCT** | intra-ligand charge transfer |
| **IPCE** | Incident photon to current efficiency conversion |
| **ISC** | intersystem crossing |
| **ITO** | indium tin oxide |
| $\mathbf{j_{sc}}$ | short-circuit photocurrent density |
| **KS** | Kohn-Sham |
| **LC** | ligand-centered |
| **LCD** | liquid crystal displays |
| **LED** | light-emitting diode |
| **LLCT** | ligand to ligand charge transfer |
| **LMMCT** | ligand to metal-metal charge transfer |
| **LR** | linear response |
| **LR-TDDFT** | linear response time-dependent density functional theory |
| **LRC** | long-range corrected |
| **LUMO** | lowest unoccupied molecular orbital |
| **MECP/MECI** | minimum energy crossing point / conical intersection |
| **MLCT** | metal to ligand charge transfer |
| **MLLCT** | metal-ligand to ligand charge transfer |
| **MM** | molecular mechanics |
| **MMLCT** | metal-metal to ligand charge transfer |
| **MO** | molecular orbital |
| **MRCC** | multireference coupled cluster |
| **MRCI** | multireference configuration interaction |
| **MW** | microwave |
| **NHE** | normal hydrogen electrode |
| **NMV** | normal mode of vibration |
| **NTO** | natural transition orbital |
| **OLED** | organic-light emitting diode |
| **ONIOM** | our own N-layered integrated molecular orbital + molecular mechanics |

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|---|---|
| **OPVs** | organic photovoltaics |
| **PES** | potential energy surface |
| **PL** | photoluminescence |
| **ppy** | 2-phenylpyridine |
| **PV** | photovoltaic |
| **QM** | quantum mechanics |
| **QM/MM** | quantum mechanics/molecular mechanics |
| **RACI** | restricted access to a conical intersection |
| **RI** | resolution of the identity |
| **RIM** | restriction of internal motion |
| **RIR** | restriction of internal rotations |
| **RIV** | restriction of internal vibrations |
| **SB** | Schiff base |
| **SBCT** | symmetry-breaking charge transfer |
| **SF-DFT** | spin-flip density functional theory |
| **SOC** | spin-orbit coupling |
| **SOS** | scaled opposite spin |
| **SR** | scalar relativistic |
| **SS** | state-specific |
| **TCO** | transparent conduction oxide |
| **TDA** | Tamm-Dancoff approximation |
| **TDDFT** | time-dependent density functional theory |
| **TDHF** | time-dependent Hartree-Fock |
| **TFA** | trifluoroacetic acid |
| **THBA** | 10,10′,11,11′-tetrahydro-5,5′-bidibenzo[a,d][7]-annulenylidene |
| **THF** | tetrahydrofuran |
| **TICT** | twisted intramolecular charge transfer |
| **TPE** | tetraphenylethylene |
| **TS** | transition state |
| **$V_{oc}$** | open-circuit photovoltage |
| **xc** | exchange-correlation |
| **ZFS** | zero-field splitting |
| **ZORA** | zeroth order regular approximation |