Supporting Information: Accurate Prediction of the lowest excited states, S_1, T_1, and T_2, energies of Chromophores for Improving Solar Cell Applications

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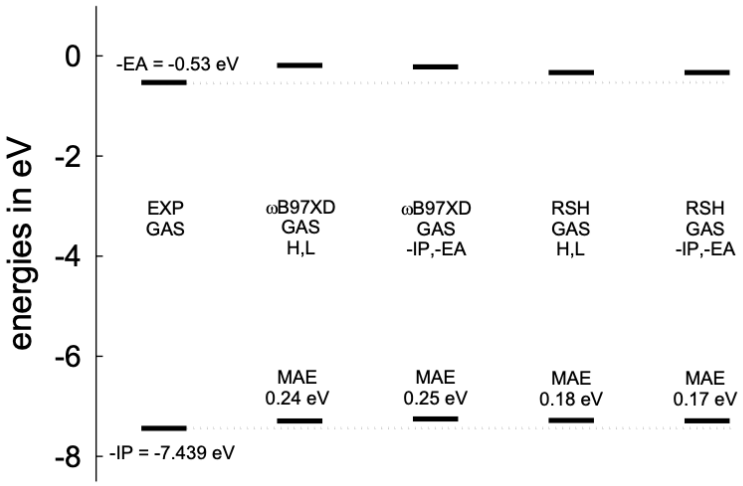
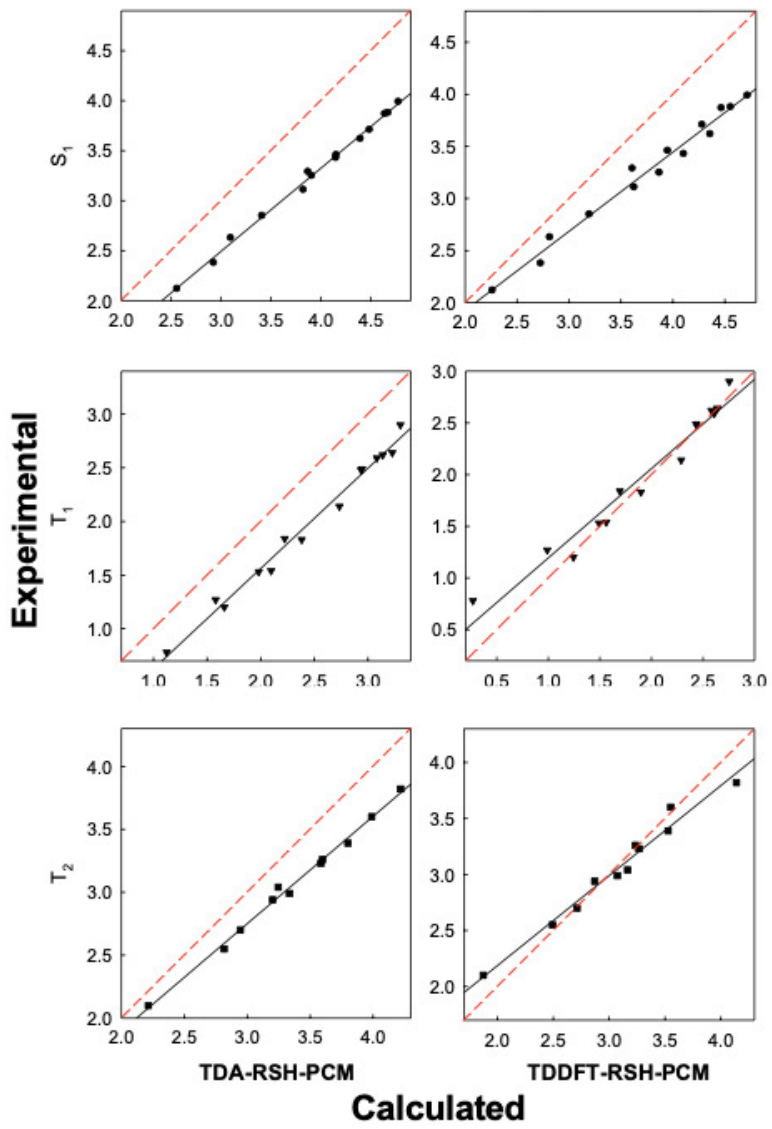
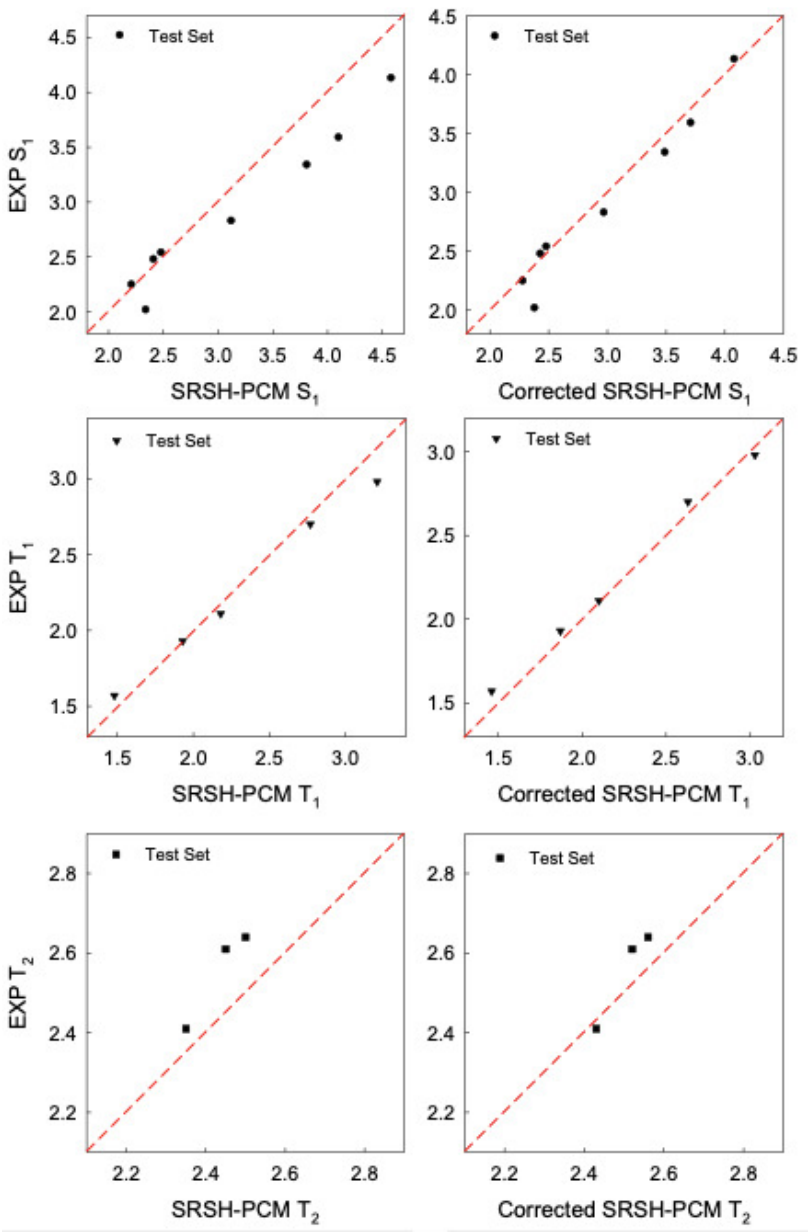


SI Figure S1. Anthracene gas phase-calculated HOMO, LUMO (H,L) energies, and -IP,-EA energies, compared to experimental IP[55]/EA[56] with corresponding MAEs listed (eV). (References follow the publication bibliography.)



SI Figure S2. RSH-PCM correlation plots of the calculated excitation energies (eV) to the experimental data for the training set molecules. (Red dashed lines of y = x lines represent the perfect fit for comparison.)



SI Figure S3. SRSH-PCM correlation plots of the calculated excitation energies (eV) to the experimental data for the test set molecules. (Red dashed lines of y = x lines represent the perfect fit for comparison.)

SI Table S1. Experimental S_1, T_1, and T_2 energies∗

Molecule	**S_1 (eV)**	**T_1 (eV)**	**T_2 (eV)**
Training set			
Naphthalene	$3.99^{(a)}$	$2.62^{(a)}$	$3.82^{(b)}$
Anthracene	$3.29^{(a)}$	$1.84^{(a)}$	$3.23^{(c)}$
Tetracene	$2.63^{(a)}$	$1.27^{(a)}$	$2.55^{(d)}$
Pentacene	$2.12^{(a)}$	$0.78^{(a)}$	$2.10^{(e)}$
Perylene	$2.85^{(a)}$	$1.53^{(a)}$	$2.99^{(f)}$
3,4,9,10-Perylenetetracarboxylic diimide (PDI)	$2.38^{(a)}$	$1.20^{(a)}$	$2.7^{(g)}$
Quinoxaline	$3.25^{(a)}$	$2.64^{(a)}$	$3.04^{(h)}$
(E,E)-1,4-Diphenyl-1,3-butadiene (DPB)	$3.46^{(a)}$	$1.83^{(a)}$	$3.26^{(i)}$
1,6-Diphenyl-1,3,5-hexatriene (DPH)	$3.11^{(a)}$	$1.54^{(a)}$	$2.94^{(i)}$
(E)-Stilbene	$3.71^{(a)}$	$2.14^{(a)}$	$3.60^{(i)}$
Chrysene	$3.43^{(a)}$	$2.48^{(a)}$	-
1-Cyanonaphthalene	$3.87^{(a)}$	$2.49^{(a)}$	-
Triphenylene	$3.62^{(a)}$	$2.90^{(a)}$	$3.39^{(j)}$
1-Methoxynaphthalene	$3.88^{(a)}$	$2.59^{(a)}$	-
Testing set			
Pyrene	$3.34^{(a)}$	$2.11^{(a)}$	-
Phenanthrene	$3.59^{(a)}$	$2.70^{(a)}$	-
Porphyrin	$2.02^{(a)}$	$1.57^{(a)}$	-
Dibenzofuran	$4.13^{(a)}$	$2.98^{(a)}$	-
Phenazine	$2.83^{(a)}$	$1.93^{(a)}$	-
TCT	$2.25^{(k)}$	-	$2.41^{(k)}$
DCT	$2.48^{(k)}$	-	$2.61^{(k)}$
MCT	$2.54^{(k)}$	-	$2.64^{(k)}$

(a) in non-polar solvent.[28]
(b) in benzene ($\varepsilon = 2.27$).[29]
(c) in solution.[30]
(d) in benzene.[31]
(e) in p-terphenyl (ε = 2.95-3.2).[32]
(f) in acetonitrile ($\varepsilon = 37.5$).[33]
(g) medium not reported.[34]
(h) medium not reported.[35]
(i) in supersonic N_2 jet ($\varepsilon = 1.47$ for liquid N_2).[36]
(j) in n-octane ($\varepsilon = 1.95$).[37]
(k) in toluene ($\varepsilon = 2.38$).[38]
∗ References follow the publication bibliography

SI Table S2. Dielectric constants associated with organic materials in a crystal phase.

Molecule	ε
Naphthalene	2.87 [52]
Anthracene	3.12 [52]
Pentacene	3.60 [53]
Perylene	3.34 [52]
Chrysene	3.09 [52]
Pyrene	3.14 [52]
quinoxaline	2.30 [54]

SI Table S3. Anthracene excited state energies (Ener.) in eV, significant orbital transitions, and oscillator strengths (Osc.) in a.u. (Oscillator strengths of triplet states are zero due to spin-forbidden vertical transitions.) H: HOMO, L: LUMO

Level	Functional	S_1			T_1		T_2	
		Ener.	Orbital Transitions	Osc.	Ener.	Orbital Transitions	Ener.	Orbital Transitions
TDA	ωB97X-D-GAS	3.901	H→L (95%), H-1→L+1 (5%)	0.116	2.307	H→L (100%)	3.677	H-1→L (54%), H→L+1 (46%)
TDDFT	ωB97X-D-GAS	3.638	H→L (100%)	0.079	1.855	H→L (96%) , H-2→L+2 (4%)	3.405	H-2→L (54%), H→L+2 (46%)
TDA	ωB97X-D-PCM	3.890	H→L (95%), H-1→L+1 (5%)	0.116	2.312	H→L (100%)	3.683	H-1→L (54%), H→L+1 (46%)
TDDFT	ωB97X-D-PCM	3.638	H→L (100%)	0.079	1.864	H→L (96%) , H-2→L+2 (4%)	3.413	H-2→L (54%), H→L+2 (46%)
TDA	RSH-GAS	3.870	H→L (95%), H-1→L+1 (5%)	0.111	2.218	H→L (100%)	3.575	H-2→L (54%), H→L+2 (46%)
TDDFT	RSH-GAS	3.608	H→L (100%)	0.075	1.680	H→L (94%) H-1→L+1 (3%) , H-2→L+2 (3%)	3.252	H-2→L (54%), H→L+2 (46%)
TDA	RSH-PCM	3.870	H→L (95%), H-1→L+1 (5%)	0.111	2.224	H→L (100%)	3.589	H-2→L (54%), H→L+2 (46%)
TDDFT	RSH-PCM	3.608	H→L (100%)	0.075	1.694	H→L (94%), H-1→L+1 (3%), H-2→L+2 (3%)	3.267	H-2→L (54%), H→L+2 (46%)
TDA	SRSH-PCM	3.551	H→L (100%)	0.082	2.156	H→L (100%)	3.561	H-2→L (57%), H→L+2 (43%)
TDDFT	SRSH-PCM	3.330	H→L (100%)	0.054	1.836	H→L (100%)	3.323	H-2→L (56%), H→L+2 (44%)

SI Table S4. Anthracene RSH-PCM excited state energies (eV) at various solvents parameterized by the scalar dielectric constant (ε). Also listed is the solvent refractive index (n_D).

Solvent			S_1		T_1		T_2	
Name	ε	n_D	TDA	TDDFT	TDA	TDDFT	TDA	TDDFT
Cyclohexane	2.02	1.426	3.868	3.608	2.221	1.690	3.581	3.262
Benzene	2.27	1.501	3.868	3.608	2.221	1.691	3.582	3.264
Solid State	3.50	1.400	3.868	3.608	2.223	1.694	3.585	3.267
Anisole	4.33	1.517	3.868	3.608	2.223	1.696	3.586	3.269
Chloroform	4.81	1.446	3.868	3.608	2.224	1.696	3.586	3.269
Chlorobenzene	5.62	1.525	3.868	3.608	2.224	1.697	3.587	3.270
THF	7.58	1.407	3.868	3.608	2.224	1.698	3.588	3.271
DCM	8.93	1.424	3.868	3.608	2.225	1.698	3.588	3.272

SI Table S5. SRSH-PCM excited state energies (eV).

Molecule	S_1		T_1		T_2	
	TDA	TDDFT	TDA	TDDFT	TDA	TDDFT
Naphthalene	4.610	4.513	3.095	2.756	4.097	4.035
Anthracene	3.549	3.330	2.155	1.836	3.559	3.323
Tetracene	2.777	2.543	1.508	1.160	2.778	2.543
Pentacene	2.236	1.993	1.048	0.613	2.169	1.925
Perylene	3.160	2.944	1.872	1.587	3.241	3.084
PDI	2.741	2.523	1.560	1.324	2.895	2.739
Quinoxaline	3.594	3.578	3.000	2.831	3.129	2.957
DPB	3.942	3.719	2.308	1.984	3.557	3.291
DPH	3.615	3.393	2.022	1.677	3.160	2.919
(E)-Stilbene	4.271	4.055	2.655	2.352	3.965	3.643
Chrysene	3.906	3.878	2.872	2.548	3.499	3.253
1-Cyanonaphthalene	4.261	4.158	2.882	2.576	3.858	3.796
Triphenylene	4.134	4.119	3.263	2.873	3.683	3.503
1-Methoxynaphthalene	4.328	4.243	3.014	2.725	3.854	3.810

SI Table S6. RSH-PCM excited state energies (eV).

Molecule	S_1		T_1		T_2	
	TDA	TDDFT	TDA	TDDFT	TDA	TDDFT
Naphthalene	4.774	4.716	3.138	2.581	4.219	4.139
Anthracene	3.868	3.608	2.223	1.694	3.585	3.267
Tetracene	3.094	2.814	1.579	0.990	2.816	2.494
Pentacene	2.556	2.262	1.122	0.270	2.214	1.874
Perylene	3.407	3.196	1.981	1.492	3.335	3.074
PDI	2.923	2.727	1.660	1.244	2.945	2.712
Quinoxaline	3.905	3.868	3.226	2.637	3.246	3.165
DPB	4.152	3.948	2.381	1.898	3.598	3.236
DPH	3.821	3.626	2.096	1.562	3.202	2.871
(E)-Stilbene	4.484	4.280	2.734	2.288	3.988	3.551
Chrysene	4.147	4.103	2.936	2.438	3.566	3.218
1-Cyanonaphthalene	4.638	4.465	2.944	2.434	3.990	3.827
Triphenylene	4.393	4.357	3.302	2.755	3.800	3.528
1-Methoxynaphthalene	4.670	4.555	3.082	2.609	3.990	3.911

SI Table S7. SRSH-PCM excited state energies (eV) for naphthalene and tetracene with 10% reduced ω than the optimal tuned value.

Molecule(ω)	S_1		T_1		T_2	
	TDA	TDDFT	TDA	TDDFT	TDA	TDDFT
Naphthalene(216)	4.610	4.513	3.095	2.756	4.097	4.035
Naphthalene(194)	4.607	4.506	3.094	2.760	4.094	4.033
Tetracene(170)	2.777	2.543	1.508	1.160	2.778	2.543
Tetracene(153)	2.771	2.538	1.505	1.161	2.776	2.542