Exploring the Excited-States of Squaraine Dyes with TD-DFT, SOS-CIS(D) and ADC(2): Supplementary Materials

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Additional geometrical parameters

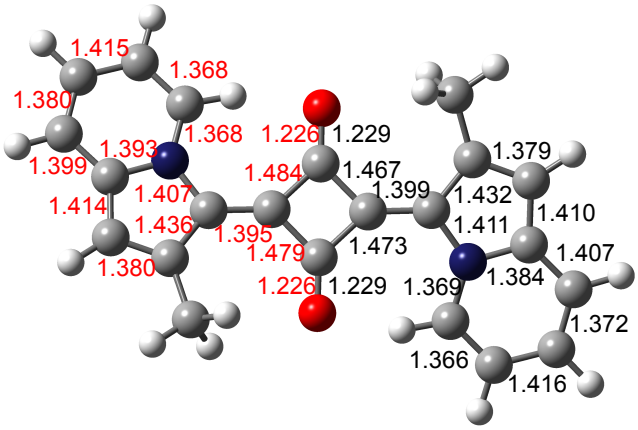
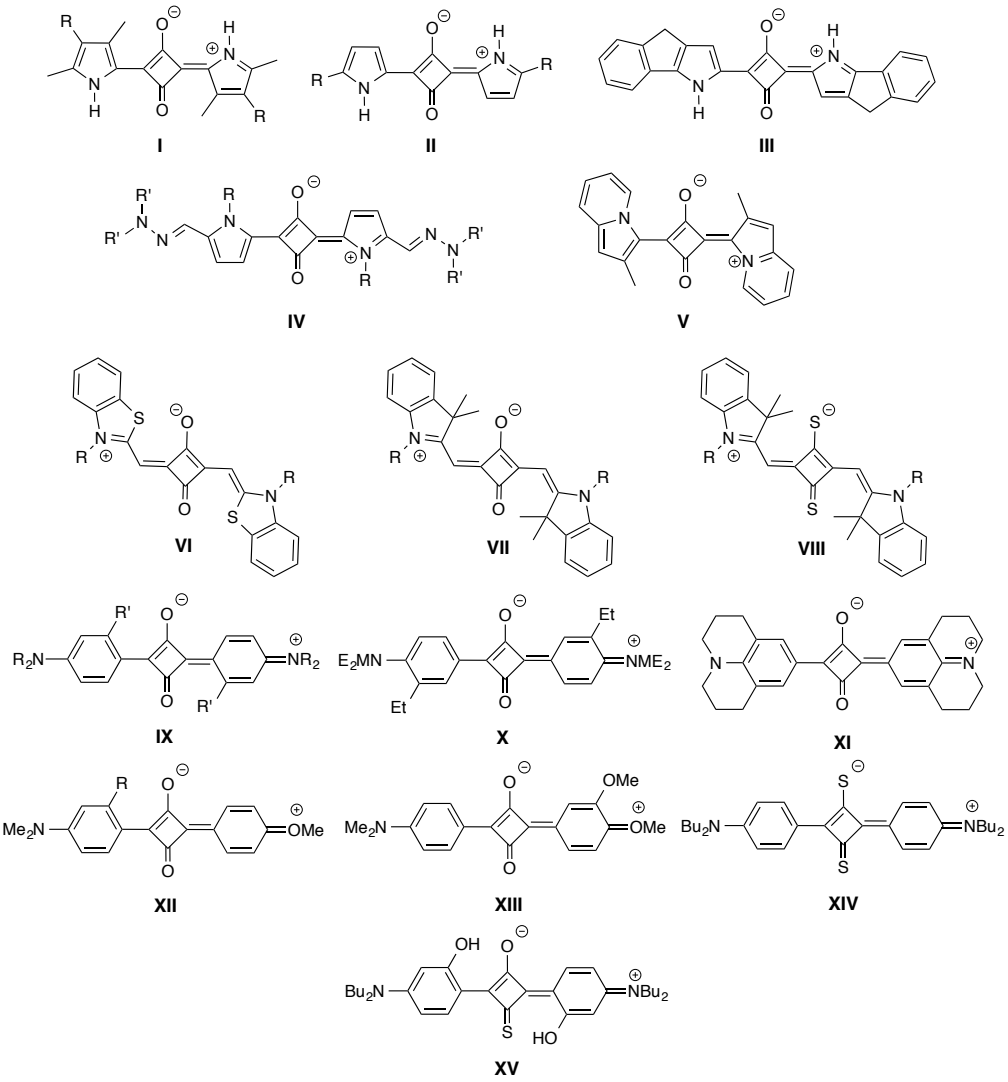


Figure S-1: Selected (TD-)DFT bond lengths for the GS (in black, on the r.h.s.) and ES (in right on the l.h.s.) for one of the two dyes represented in Figure 1 in the main text.

Complete data set for vertical absorption



Scheme 1: Representation of the dyes reported in Table S-I.

Table S-I: Comparison between theoretical 0-0 energies and experiment λ_{max}. All values in eV. Experimental references taken from Refs. 1–9

Molecule	Substituents	Solvent	Exp.	TD-DFT	SOS-CIS(D)	ADC(2)
I	R=Et	$CHCl_3$	2.214	2.526	2.019	2.154
	R=COMe	CH_2Cl_2	2.183	2.526	2.007	2.117
		CH_3CN	2.194	2.533	2.013	2.123
II	R=Naphthyl	$CHCl_3$	2.023	2.282	1.848	1.945
	R=Ph	$CHCl_3$	1.996	2.305	1.835	1.968
	R=*m*-OMe-Ph	$CHCl_3$	1.987	2.300	1.830	1.959
	R=*p*-OMe-Ph	$CHCl_3$	1.928	2.238	1.750	1.888
	R=CH=CH-Ph	$CHCl_3$	1.784	2.068	1.672	1.771
III		$CHCl_3$	1.896	2.241	1.735	1.927
IV	R=Me; R'=Ph	CH_2Cl_2	1.703	2.012	1.552	1.541
	R=PEG; R'=Me	CH_2Cl_2	1.802	2.097	1.634	1.678
V		CH_2Cl_2	1.813	2.133	1.539	1.694
VI	R=Me	MeOH	1.916	2.249	1.638	1.741
	R=Et	MeOH	1.907	2.234	1.615	1.721
VII	R=CH_2PhCOOH	H_2O	1.922	2.297	1.664	1.718
	R=*n*Pr	CH_2Cl_2	1.949	2.320	1.704	1.754
	R=*n*Bu	CH_2Cl_2	1.856	2.308	1.693	1.743
VIII	R=*n*Pr	Toluene	1.829	2.109	1.540	1.620
	R=*n*Bu	Toluene	1.779	2.107	1.538	1.616
IX	R=Me; R'=H	CH_2Cl_2	1.974	2.420	1.877	1.898
	R=Et; R'=H	CH_2Cl_2	1.955	2.381	1.823	1.837
	R=*n*Pr; R'=H	CH_2Cl_2	1.941	2.368	1.811	1.820
	R=*n*Bu; R'=H	Toluene	1.949	2.354	1.803	1.800
	R=Me; R'=Me	CH_2Cl_2	1.928	2.314	1.764	1.802
	R=Et; R'=Me	CH_2Cl_2	1.904	2.277	1.712	1.744
	R=*n*Bu; R'=Me	CH_2Cl_2	1.887	2.260	1.698	1.595
	R=Me; R'=OH	CH_2Cl_2	1.949	2.410	1.773	1.838
	R=Et; R'=OH	CH_2Cl_2	1.934	2.389	1.741	1.799
	R=*n*Bu; R'=OH	CH_2Cl_2	1.913	2.364	1.721	1.769
	R=Me; R'=Et	CH_2Cl_2	1.928	2.284	1.729	1.768
	R=Me; R'=OMe	CH_2Cl_2	1.962	2.338	1.786	1.820
	R=*n*Bu; R'=OMe	CH_2Cl_2	1.927	2.301	1.739	1.769
X		CH_2Cl_2	1.968	2.365	1.880	1.849
XI		CH_2Cl_2	1.876	2.322	1.748	1.761
XII	R=H	$CHCl_3$	2.142	2.513	2.013	2.008
	R=OH	$CHCl_3$	2.180	2.565	2.026	2.022
XIII		$CHCl_3$	2.112	2.474	1.969	1.948
XIV		Toluene	1.805	2.088	1.634	1.669
XV		CH_3CN	1.876	2.291	1.681	1.732

Additional vibronic information

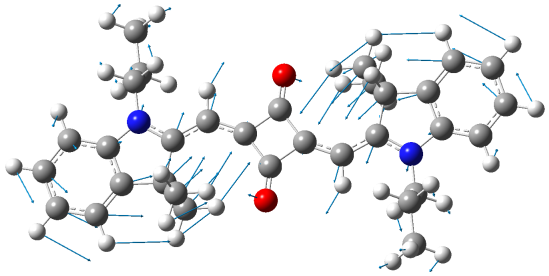


Figure S-2: Excited-state vibrational model n^o 10 of compound **4**.

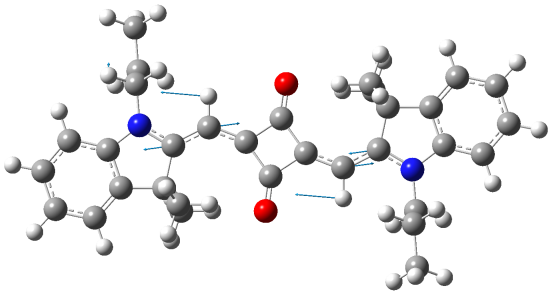


Figure S-3: Excited-state vibrational model n^o 167 of compound **4**.

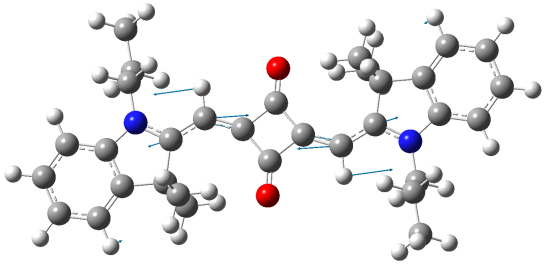


Figure S-4: Excited-state vibrational model n^o 168 of compound **4**.

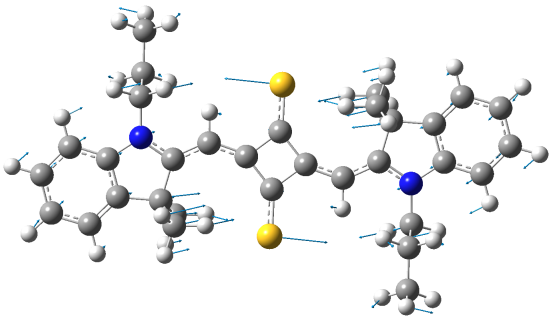


Figure S-5: Excited-state vibrational model n^o 17 of compound **5**.

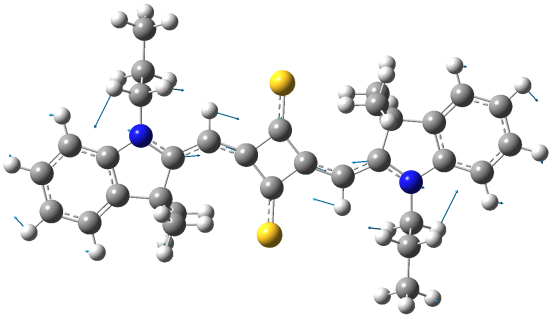


Figure S-6: Excited-state vibrational model n^o 168 of compound **5**.

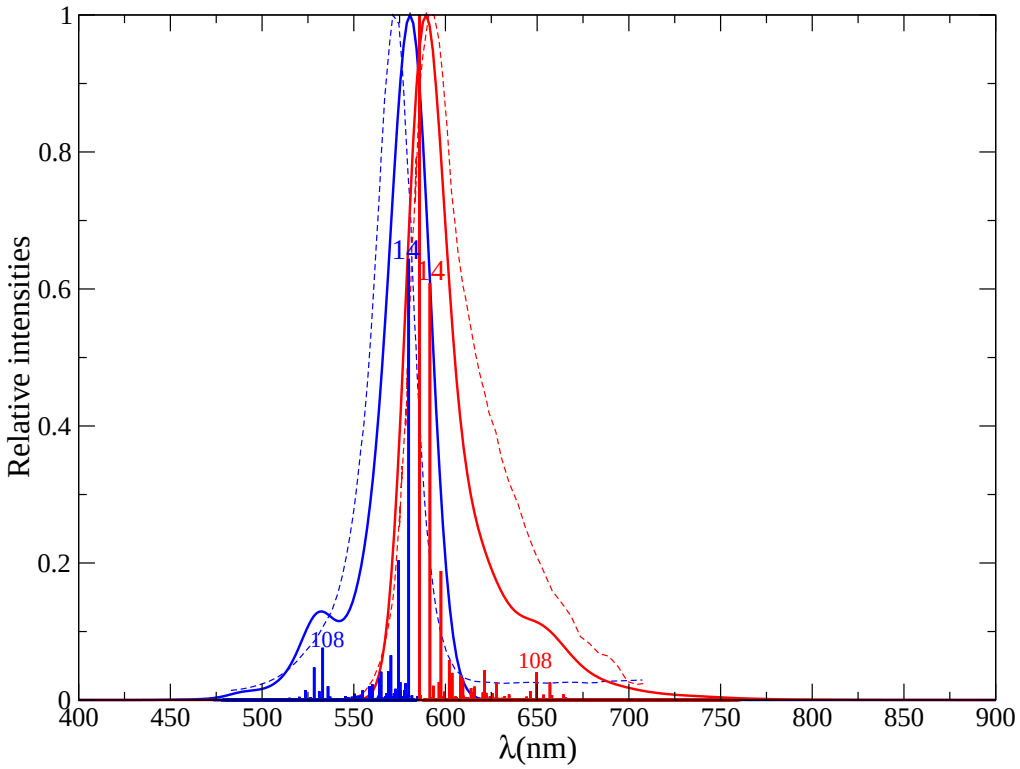


Figure S-7: Comparison between experimental (dashed lines) and theoretical (full lines and stick contribution) for compound **2**. The experimental spectra si taken from Ref. 3. The blue (red) curves correspond to the absorption (emission). The most important modes (14 and 108) are displayed in Figures S-8 and S-9.

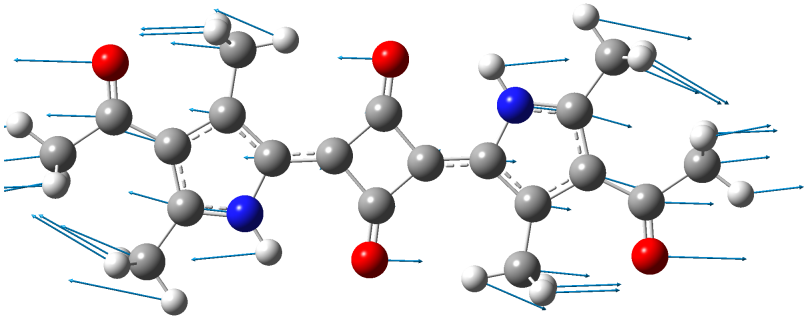


Figure S-8: Excited-state vibrational model n^o 14 of compound **2**.

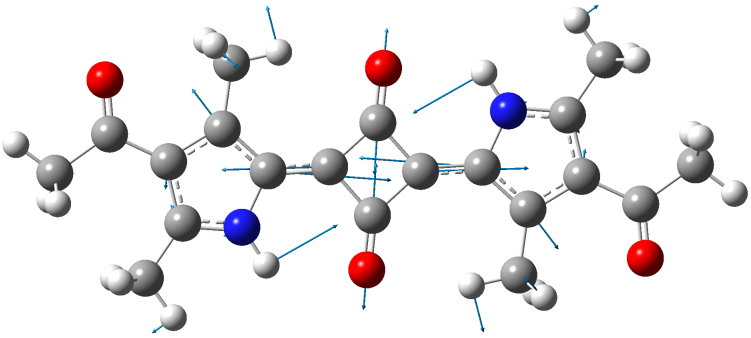


Figure S-9: Excited-state vibrational model n^o 108 of compound **2**.

References

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