Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information:

Triangulenium Dyes: the Comprehensive Photo-Absorption and Emission Story of a Versatile Family of Chromophores

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Part I

Density-Functional Benchmark

1 TATA

1.1 SVWN5

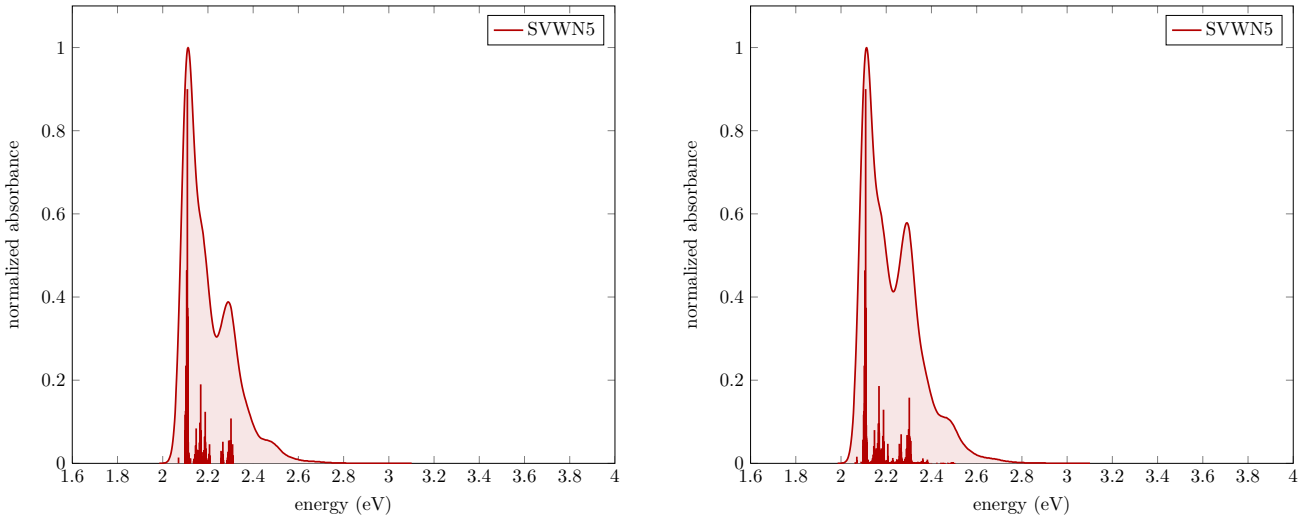

Fig. S1 UV/vis absorption spectra of TATA computed within the (left) Franck-Condon and (right) Franck-Condon-Herzberg-Teller approximations at SVWN5/6-31+G* level of theory in acetonitrile solvent. The envelope of each spectrum is obtained by a Gaussian convolution (FWHM = 250 cm^{-1}) of the vibronic transitions (sticks) betwen the S_0 and S_1 electronic states.

1.2 PBE

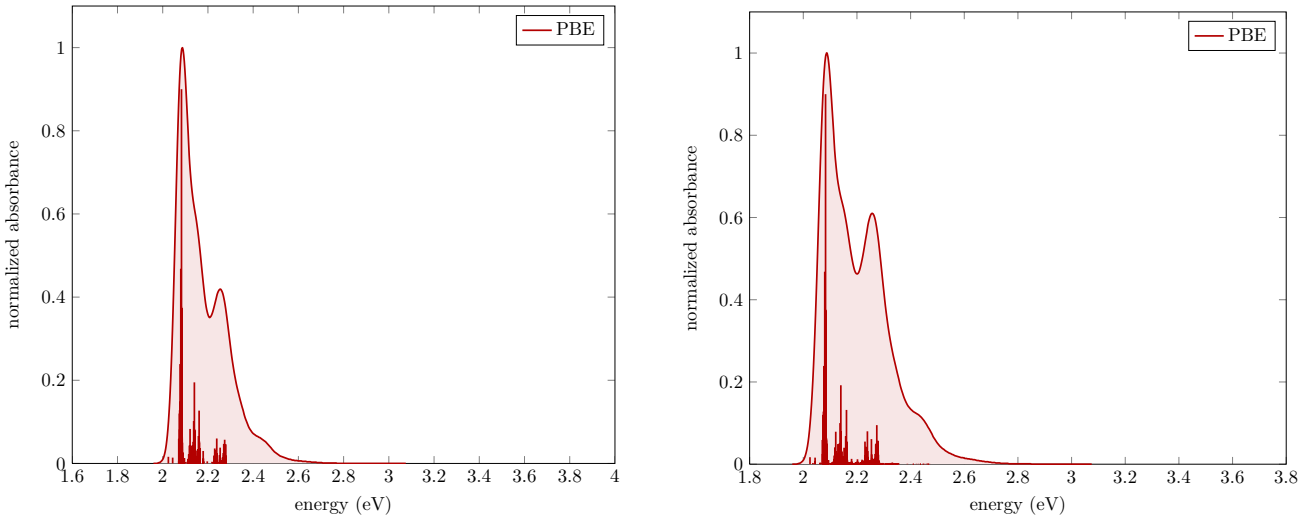

Fig. S2 UV/vis absorption spectra of TATA computed within the (left) Franck-Condon and (right) Franck-Condon-Herzberg-Teller approximations at PBE/6-31+G* level of theory in acetonitrile solvent. The envelope of each spectrum is obtained by a Gaussian convolution (FWHM = 250 cm^{-1}) of the vibronic transitions (sticks) betwen the S_0 and S_1 electronic states.

1.3 B3LYP

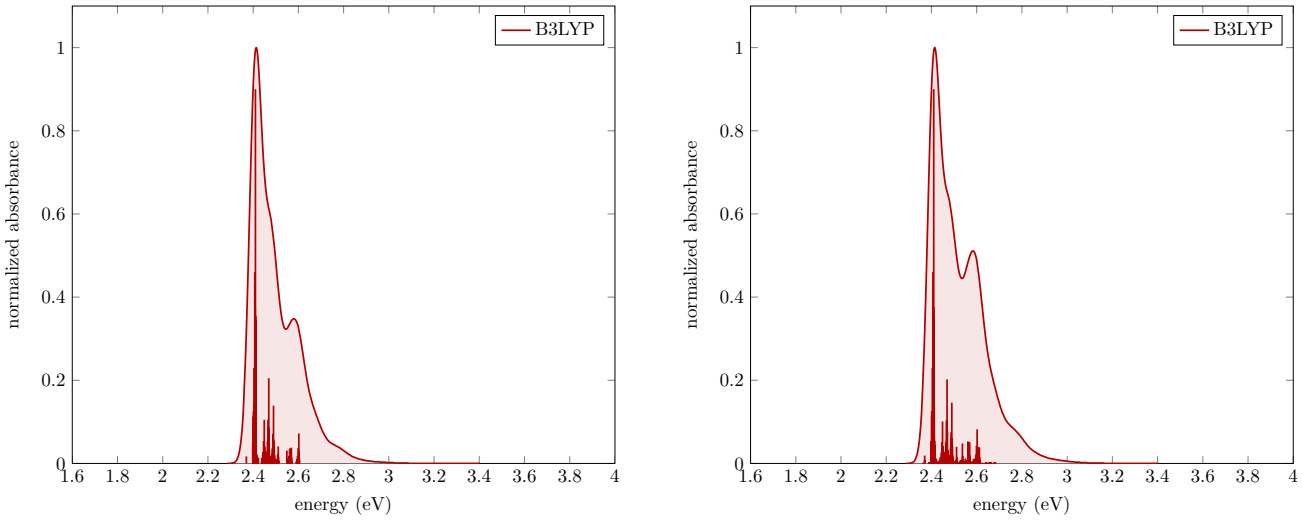

Fig. S3 UV/vis absorption spectra of TATA computed within the (left) Franck-Condon and (right) Franck-Condon-Herzberg-Teller approximations at B3LYP/6-31+G* level of theory in acetonitrile solvent. The envelope of each spectrum is obtained by a Gaussian convolution (FWHM = 250 cm^{-1}) of the vibronic transitions (sticks) betwen the S_0 and S_1 electronic states.

1.4 PBE0

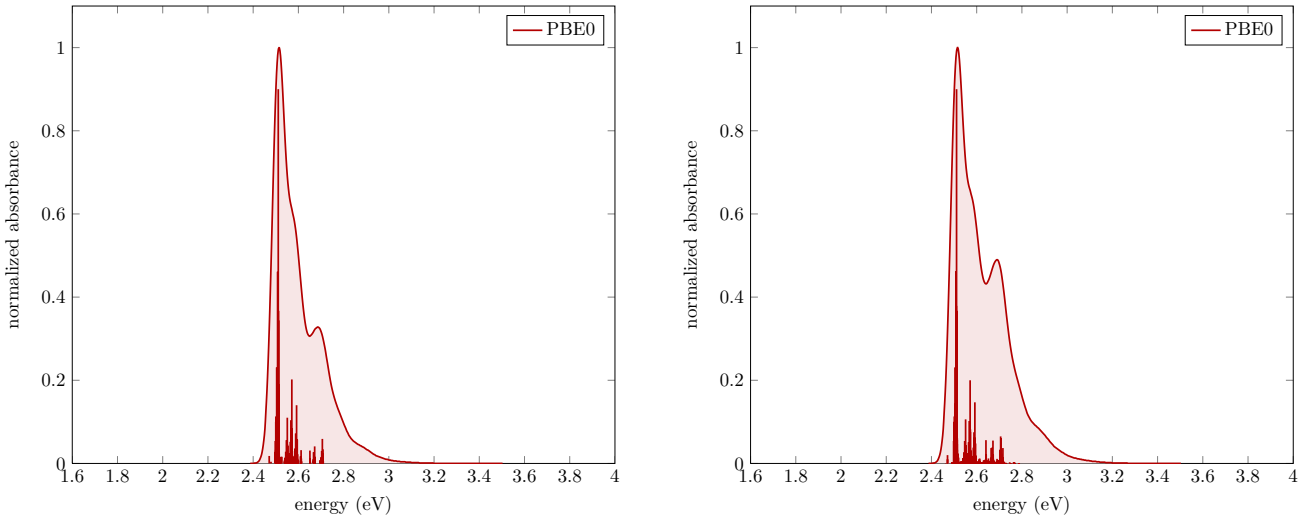

Fig. S4 UV/vis absorption spectra of TATA computed within the (left) Franck-Condon and (right) Franck-Condon-Herzberg-Teller approximations at PBE0/6-31+G* level of theory in acetonitrile solvent. The envelope of each spectrum is obtained by a Gaussian convolution (FWHM = 250 cm^{-1}) of the vibronic transitions (sticks) betwen the S_0 and S_1 electronic states.

1.5 M06

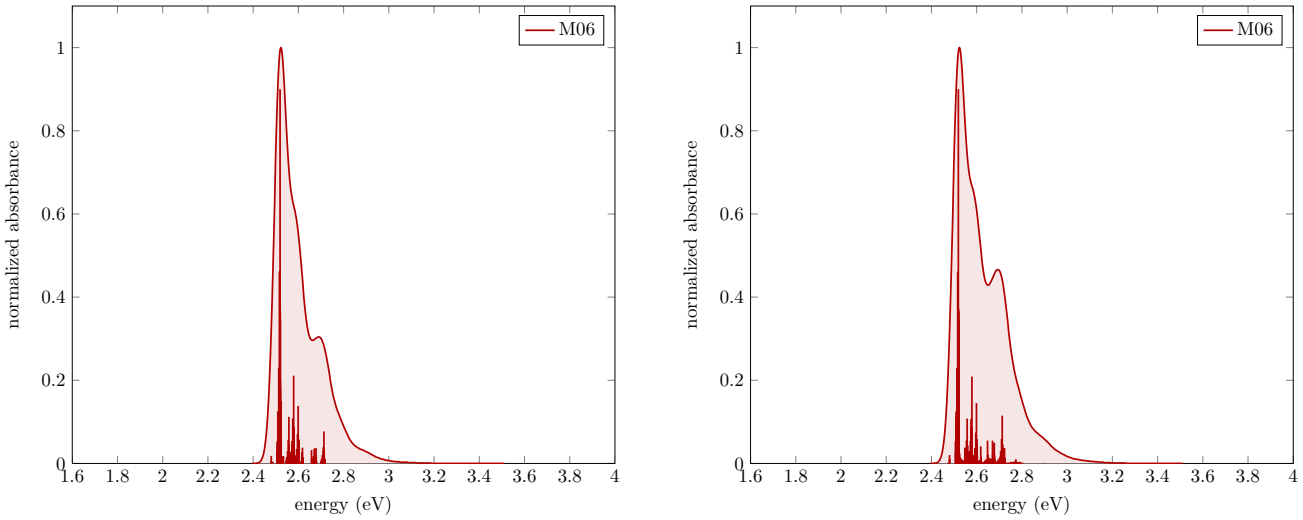

Fig. S5 UV/vis absorption spectra of TATA computed within the (left) Franck-Condon and (right) Franck-Condon-Herzberg-Teller approximations at M06/6-31+G* level of theory in acetonitrile solvent. The envelope of each spectrum is obtained by a Gaussian convolution (FWHM = 250 cm^{-1}) of the vibronic transitions (sticks) betwen the S_0 and S_1 electronic states.

1.6 BMK

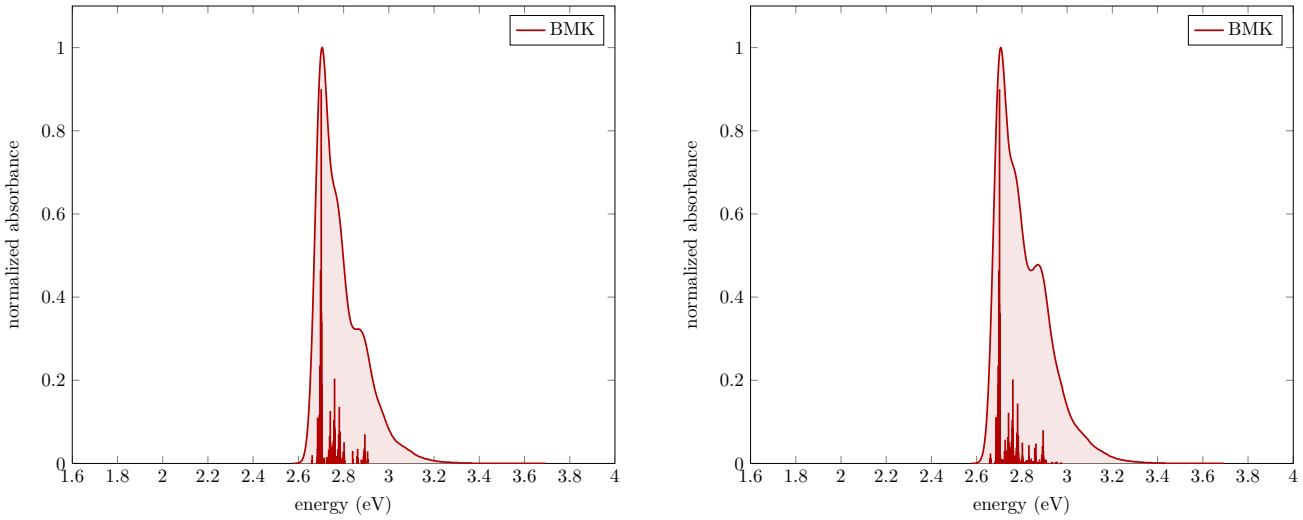

Fig. S6 UV/vis absorption spectra of TATA computed within the (left) Franck-Condon and (right) Franck-Condon-Herzberg-Teller approximations at BMK/6-31+G* level of theory in acetonitrile solvent. The envelope of each spectrum is obtained by a Gaussian convolution (FWHM = 250 cm^{-1}) of the vibronic transitions (sticks) betwen the S_0 and S_1 electronic states.

1.7 M06-2X

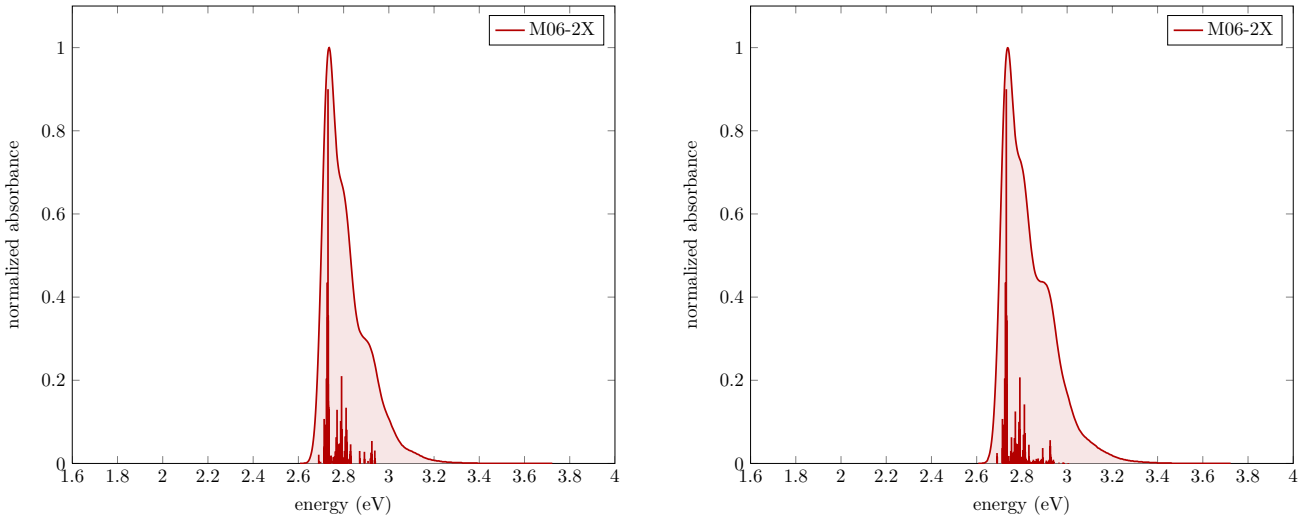

Fig. S7 UV/vis absorption spectra of TATA computed within the (left) Franck-Condon and (right) Franck-Condon-Herzberg-Teller approximations at M06-2X/6-31+G* level of theory in acetonitrile solvent. The envelope of each spectrum is obtained by a Gaussian convolution (FWHM = 250 cm^{-1}) of the vibronic transitions (sticks) betwen the S_0 and S_1 electronic states.

1.8 M06-HF

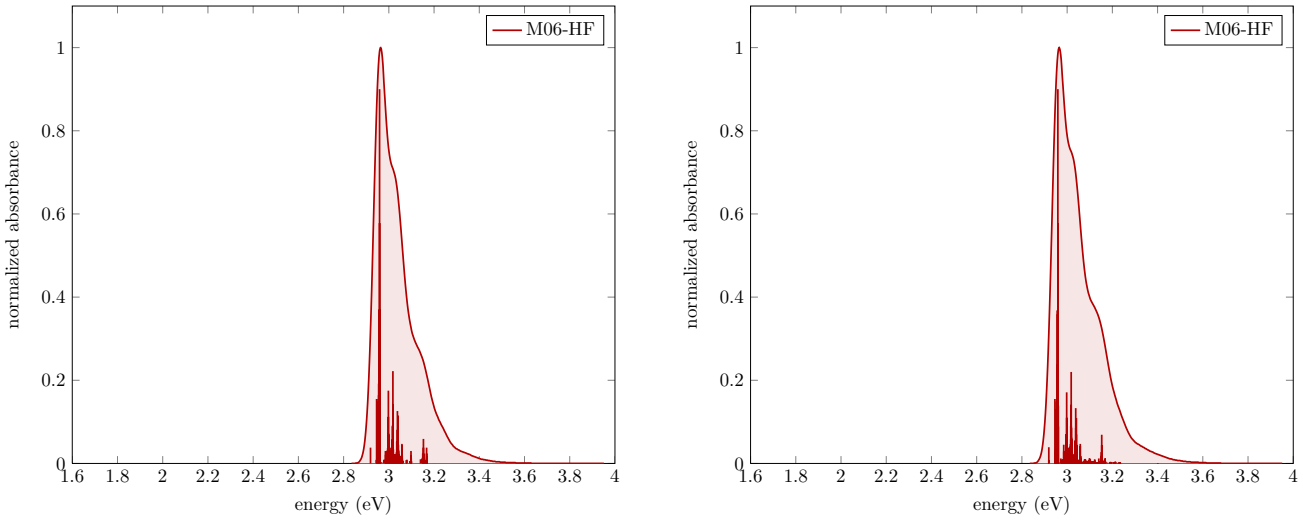

Fig. S8 UV/vis absorption spectra of TATA computed within the (left) Franck-Condon and (right) Franck-Condon-Herzberg-Teller approximations at M06-HF/6-31+G* level of theory in acetonitrile solvent. The envelope of each spectrum is obtained by a Gaussian convolution (FWHM = 250 cm^{-1}) of the vibronic transitions (sticks) betwen the S_0 and S_1 electronic states.

1.9 ωB97XD

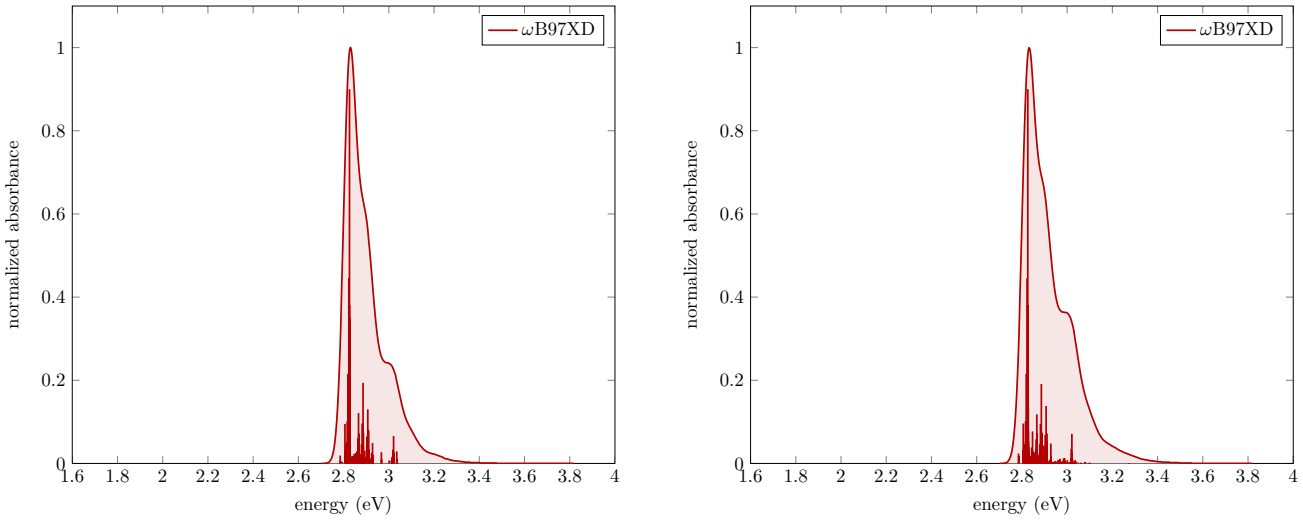

Fig. S9 UV/vis absorption spectra of TATA computed within the (left) Franck-Condon and (right) Franck-Condon-Herzberg-Teller approximations at ωB97XD/6-31+G* level of theory in acetonitrile solvent. The envelope of each spectrum is obtained by a Gaussian convolution (FWHM = 250 cm^{-1}) of the vibronic transitions (sticks) betwen the S_0 and S_1 electronic states.

1.10 CAM-B3LYP

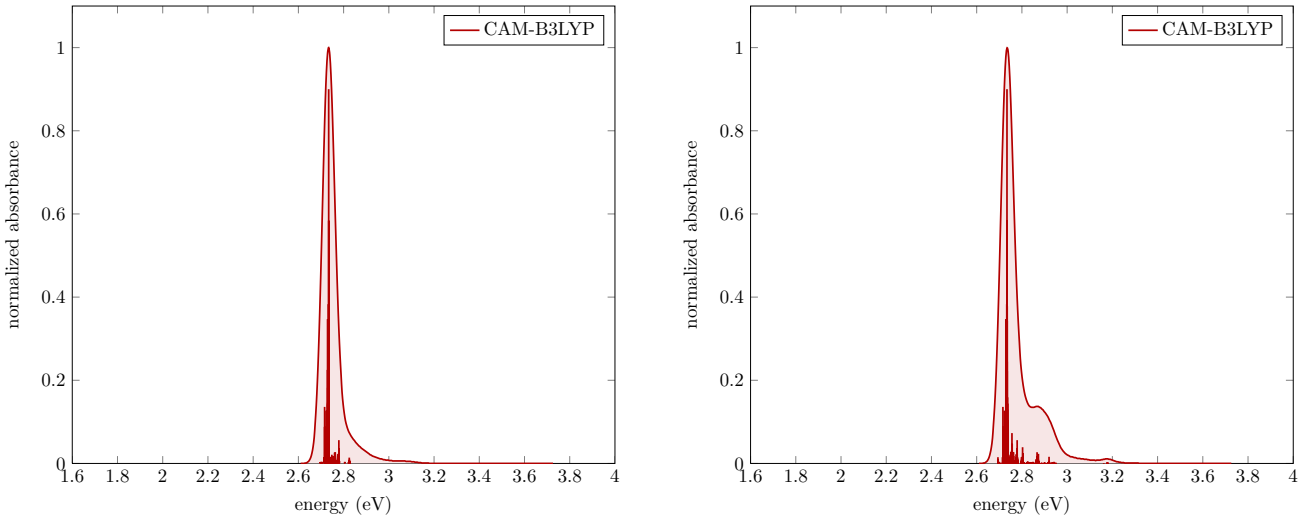

Fig. S10 UV/vis absorption spectra of TATA computed within the (left) Franck-Condon and (right) Franck-Condon-Herzberg-Teller approximations at CAM-B3LYP/6-31+G* level of theory in acetonitrile solvent. The envelope of each spectrum is obtained by a Gaussian convolution (FWHM = 250 cm^{-1}) of the vibronic transitions (sticks) betwen the S_0 and S_1 electronic states.

2 ADOTA

2.1 *SVWN5*

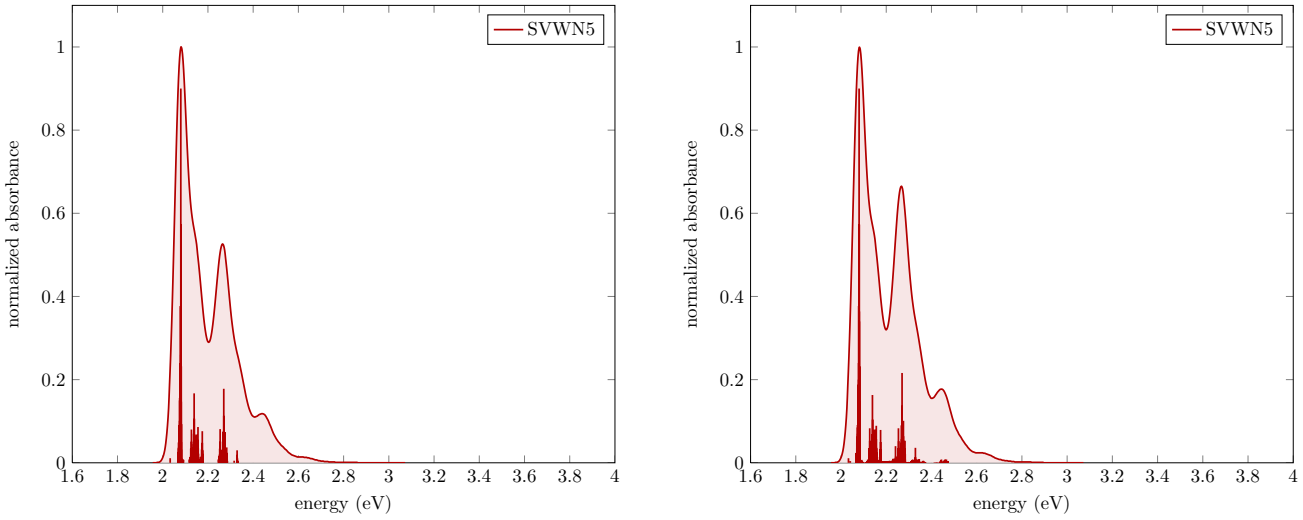

Fig. S11 UV/vis absorption spectra of ADOTA computed within the (left) Franck-Condon and (right) Franck-Condon-Herzberg-Teller approximations at SVWN5/6-31+G* level of theory in acetonitrile solvent. The envelope of each spectrum is obtained by a Gaussian convolution (FWHM = 250 cm^{-1}) of the vibronic transitions (sticks) betwen the S_0 and S_1 electronic states.

2.2 PBE

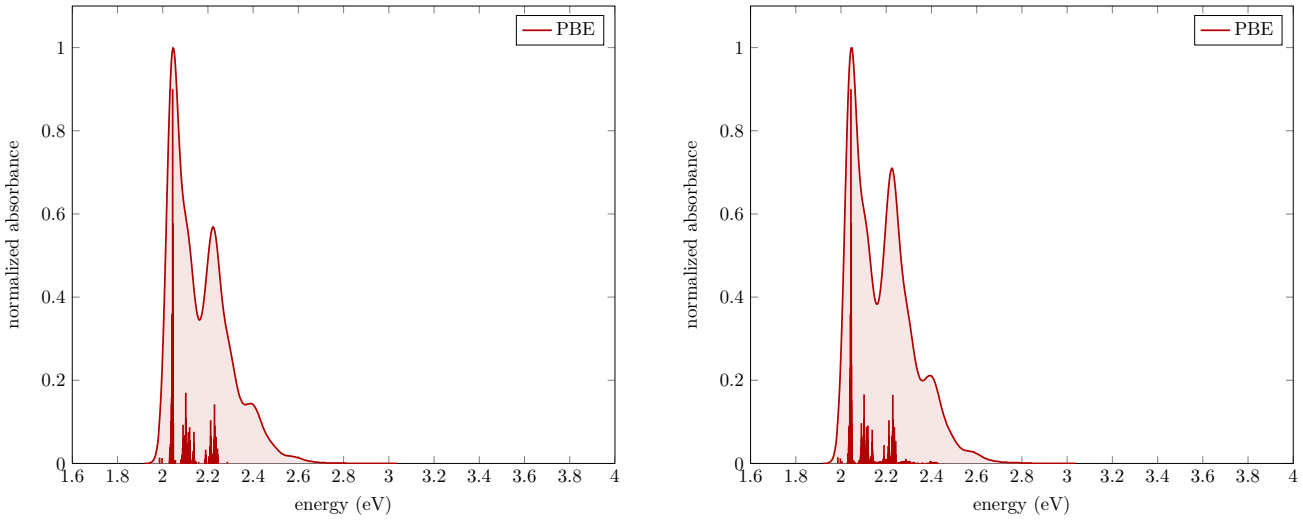

Fig. S12 UV/vis absorption spectra of ADOTA computed within the (left) Franck-Condon and (right) Franck-Condon-Herzberg-Teller approximations at PBE/6-31+G* level of theory in acetonitrile solvent. The envelope of each spectrum is obtained by a Gaussian convolution (FWHM = 250 cm^{-1}) of the vibronic transitions (sticks) betwen the S_0 and S_1 electronic states.

2.3 B3LYP

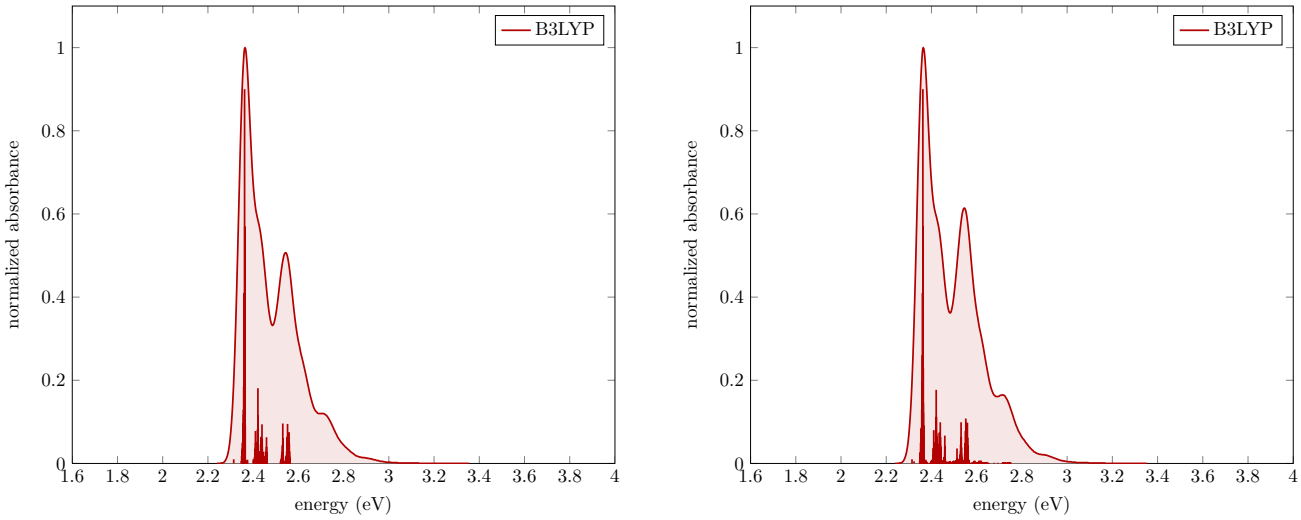

Fig. S13 UV/vis absorption spectra of ADOTA computed within the (left) Franck-Condon and (right) Franck-Condon-Herzberg-Teller approximations at B3LYP/6-31+G* level of theory in acetonitrile solvent. The envelope of each spectrum is obtained by a Gaussian convolution (FWHM = 250 cm^{-1}) of the vibronic transitions (sticks) betwen the S_0 and S_1 electronic states.

2.4 PBE0

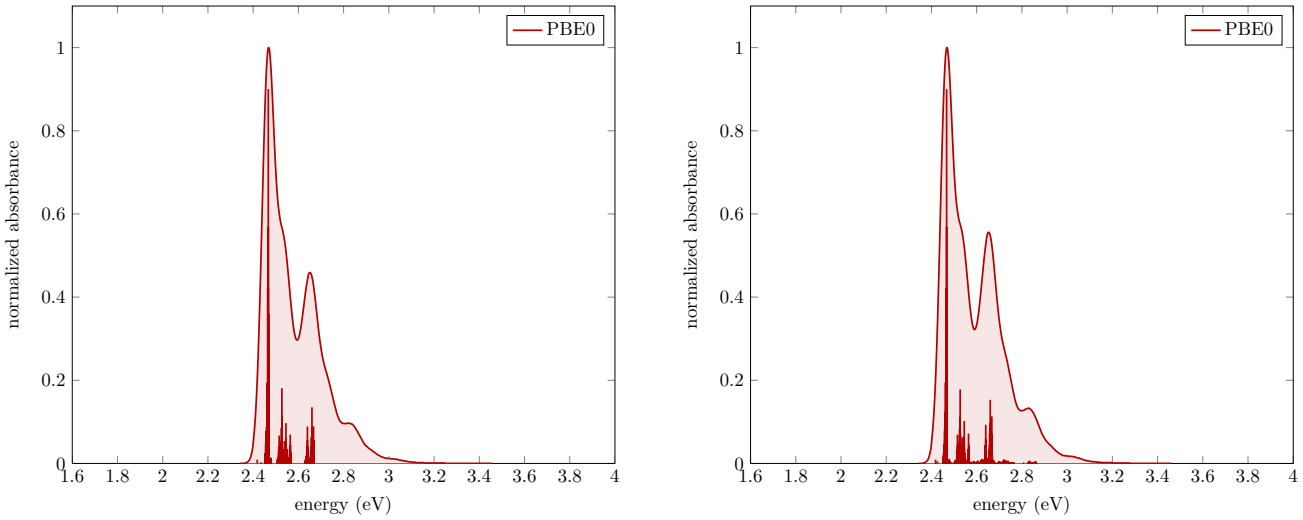

Fig. S14 UV/vis absorption spectra of ADOTA computed within the (left) Franck-Condon and (right) Franck-Condon-Herzberg-Teller approximations at PBE0/6-31+G* level of theory in acetonitrile solvent. The envelope of each spectrum is obtained by a Gaussian convolution (FWHM = 250 cm^{-1}) of the vibronic transitions (sticks) betwen the S_0 and S_1 electronic states.

2.5 M06

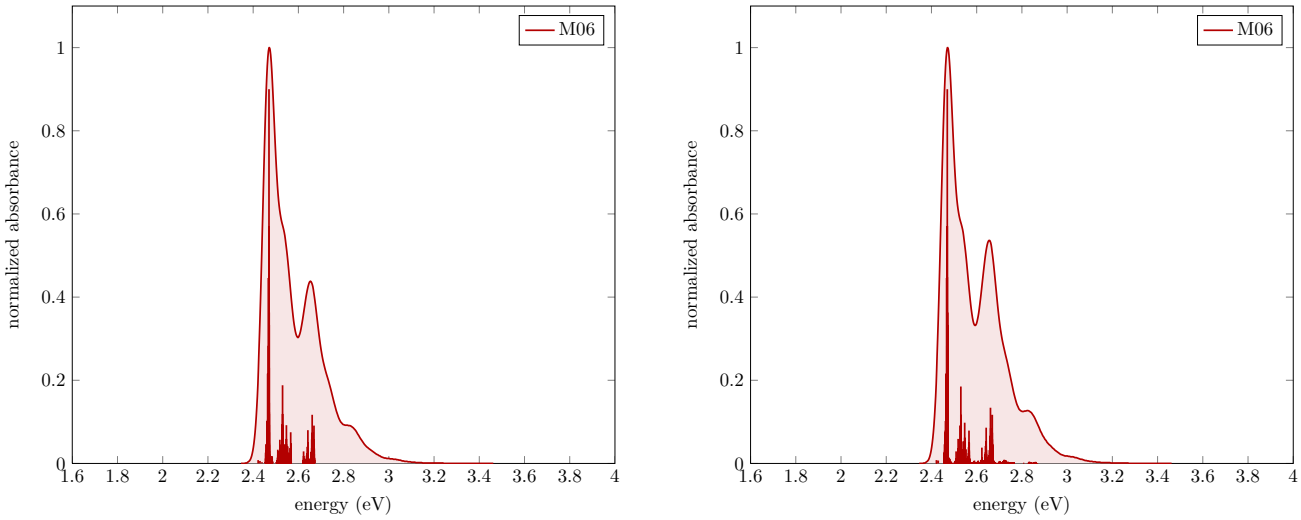

Fig. S15 UV/vis absorption spectra of ADOTA computed within the (left) Franck-Condon and (right) Franck-Condon-Herzberg-Teller approximations at M06/6-31+G* level of theory in acetonitrile solvent. The envelope of each spectrum is obtained by a Gaussian convolution (FWHM = 250 cm^{-1}) of the vibronic transitions (sticks) betwen the S_0 and S_1 electronic states.

2.6 PBE0-1/3

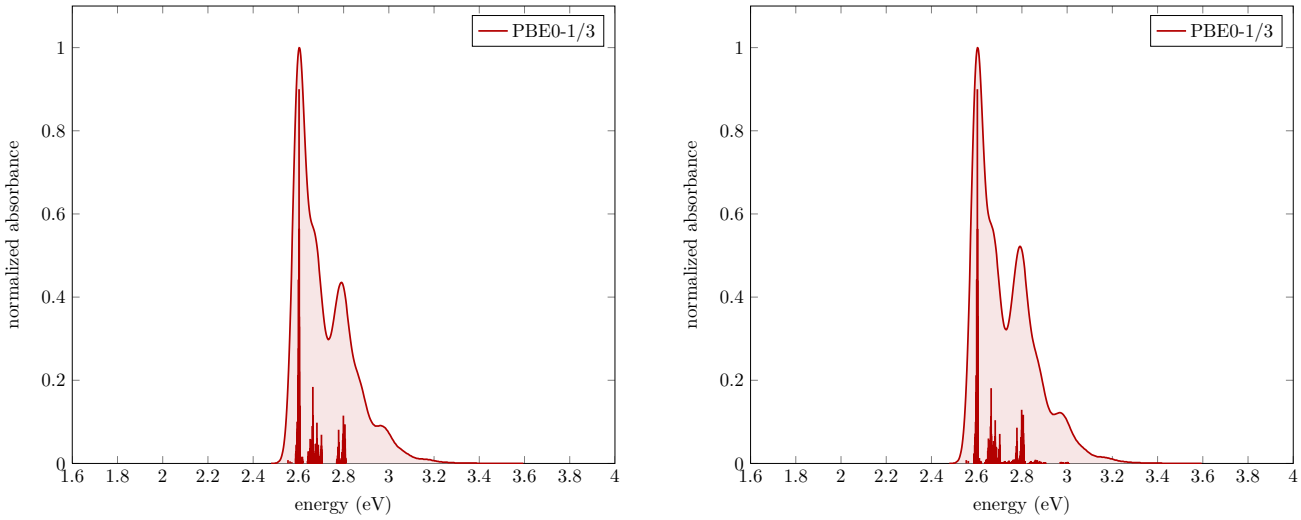

Fig. S16 UV/vis absorption spectra of ADOTA computed within the (left) Franck-Condon and (right) Franck-Condon-Herzberg-Teller approximations at PBE0-1/3/6-31+G* level of theory in acetonitrile solvent. The envelope of each spectrum is obtained by a Gaussian convolution (FWHM = 250 cm^{-1}) of the vibronic transitions (sticks) betwen the S_0 and S_1 electronic states.

2.7 BMK

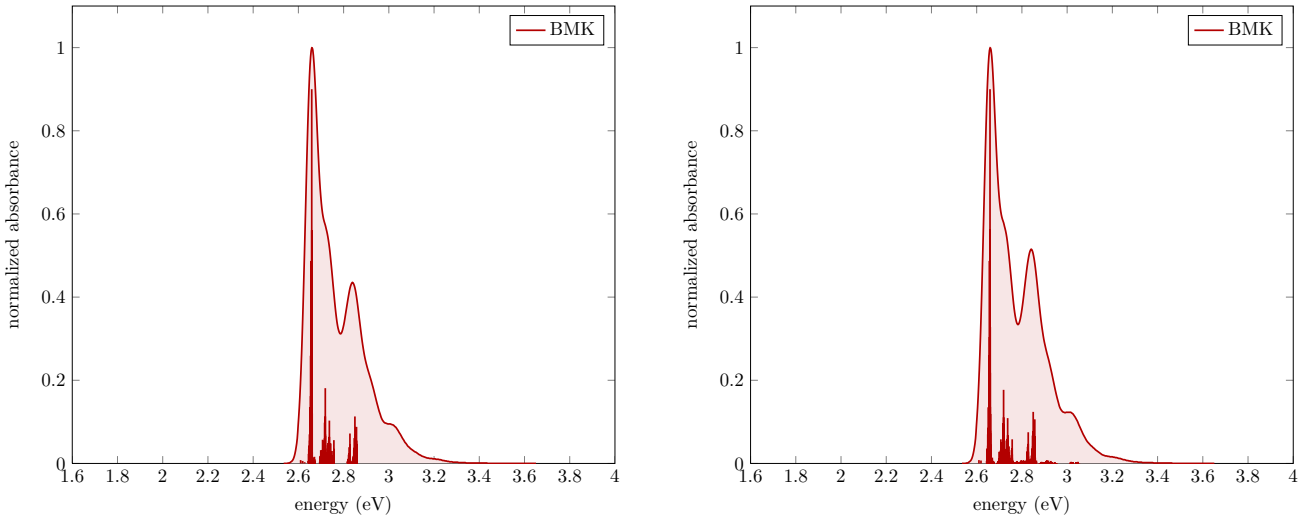

Fig. S17 UV/vis absorption spectra of ADOTA computed within the (left) Franck-Condon and (right) Franck-Condon-Herzberg-Teller approximations at BMK/6-31+G* level of theory in acetonitrile solvent. The envelope of each spectrum is obtained by a Gaussian convolution (FWHM = 250 cm^{-1}) of the vibronic transitions (sticks) betwen the S_0 and S_1 electronic states.

2.8 M06-2X

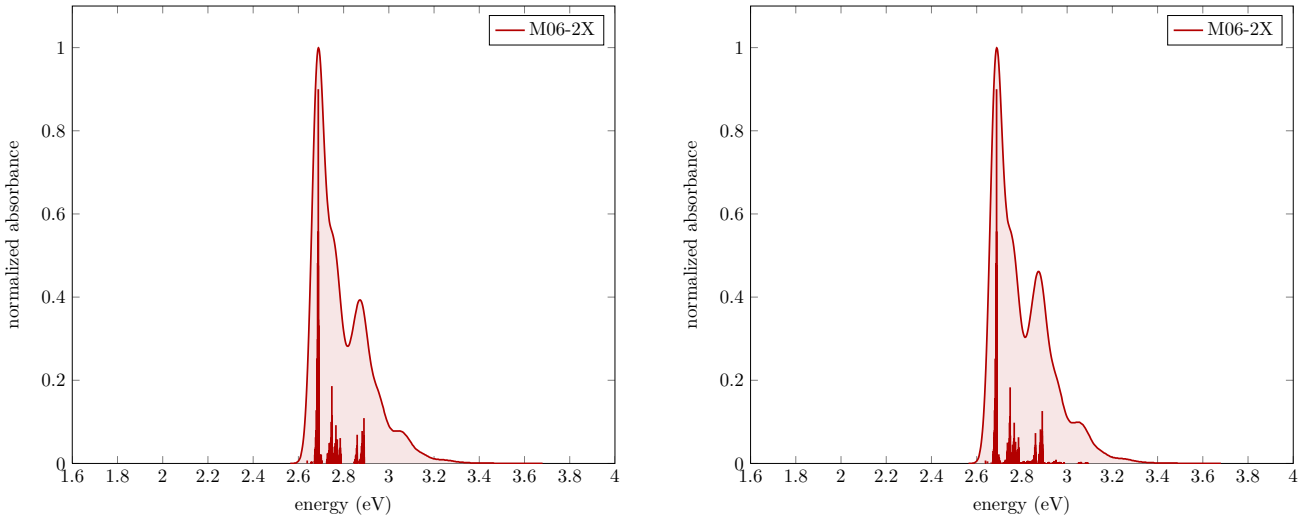

Fig. S18 UV/vis absorption spectra of ADOTA computed within the (left) Franck-Condon and (right) Franck-Condon-Herzberg-Teller approximations at M06-2X/6-31+G* level of theory in acetonitrile solvent. The envelope of each spectrum is obtained by a Gaussian convolution (FWHM = 250 cm^{-1}) of the vibronic transitions (sticks) betwen the S_0 and S_1 electronic states.

2.9 M06-HF

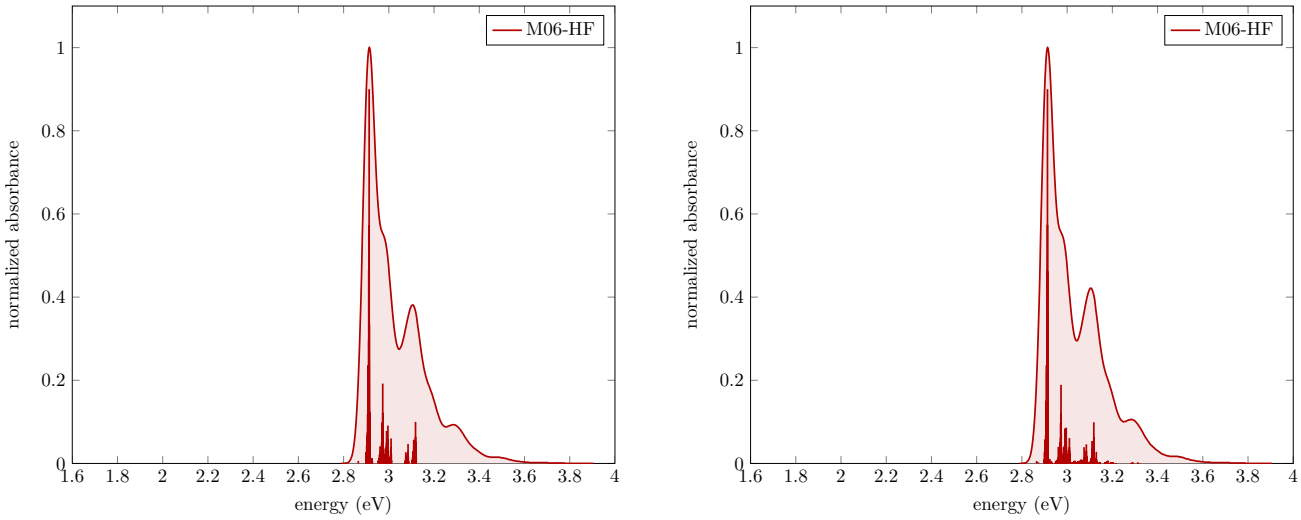

Fig. S19 UV/vis absorption spectra of ADOTA computed within the (left) Franck-Condon and (right) Franck-Condon-Herzberg-Teller approximations at M06-HF/6-31+G* level of theory in acetonitrile solvent. The envelope of each spectrum is obtained by a Gaussian convolution (FWHM = 250 cm^{-1}) of the vibronic transitions (sticks) betwen the S_0 and S_1 electronic states.

2.10 ωB97XD

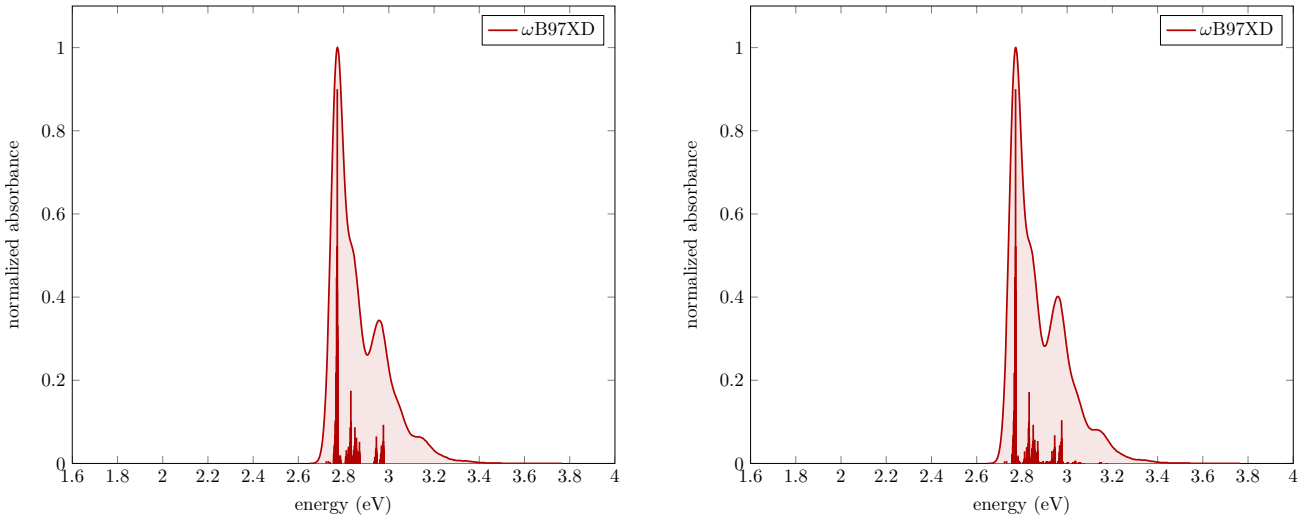

Fig. S20 UV/vis absorption spectra of ADOTA computed within the (left) Franck-Condon and (right) Franck-Condon-Herzberg-Teller approximations at ωB97XD/6-31+G* level of theory in acetonitrile solvent. The envelope of each spectrum is obtained by a Gaussian convolution (FWHM = 250 cm^{-1}) of the vibronic transitions (sticks) betwen the S_0 and S_1 electronic states.

2.11 CAM-B3LYP

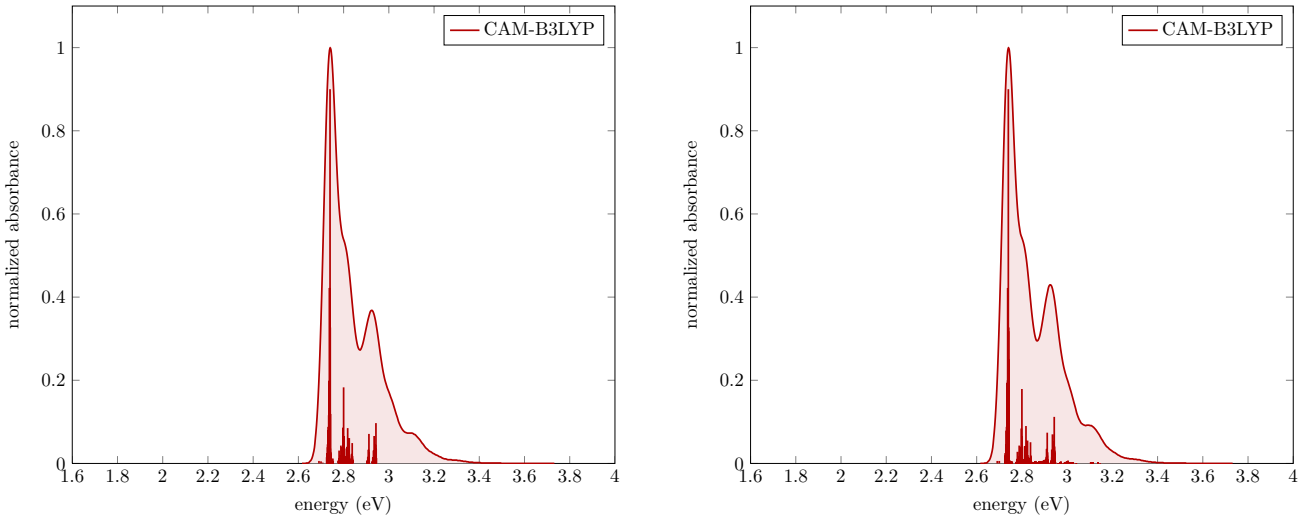

Fig. S21 UV/vis absorption spectra of ADOTA computed within the (left) Franck-Condon and (right) Franck-Condon-Herzberg-Teller approximations at CAM-B3LYP/6-31+G* level of theory in acetonitrile solvent. The envelope of each spectrum is obtained by a Gaussian convolution (FWHM = 250 cm^{-1}) of the vibronic transitions (sticks) betwen the S_0 and S_1 electronic states.

3 DAOTA

3.1 *SVWN5*

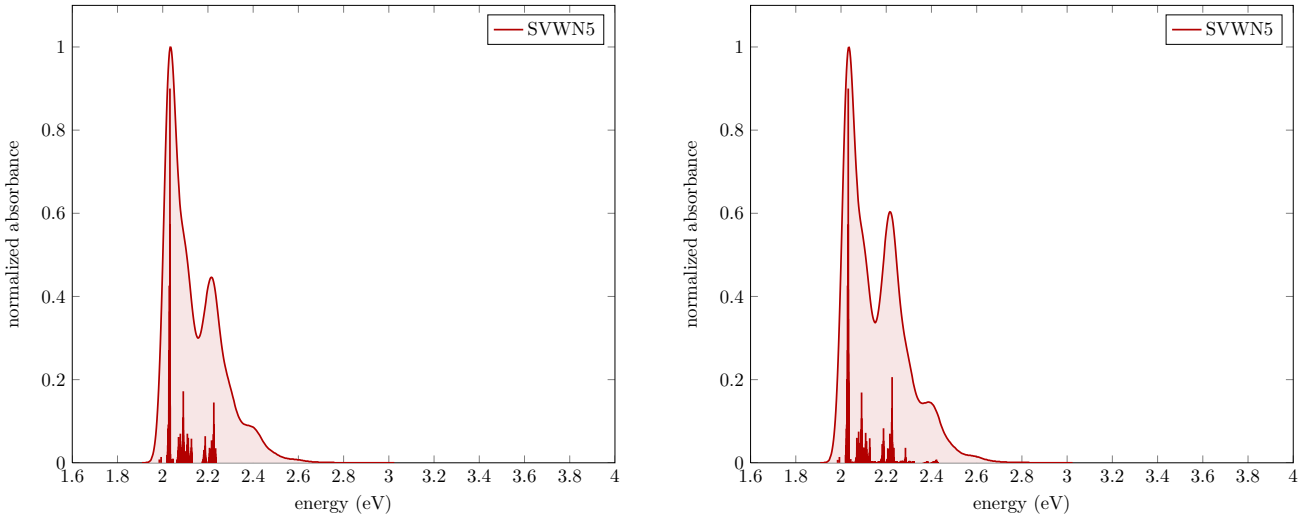

Fig. S22 UV/vis absorption spectra of DAOTA computed within the (left) Franck-Condon and (right) Franck-Condon-Herzberg-Teller approximations at SVWN5/6-31+G* level of theory in acetonitrile solvent. The envelope of each spectrum is obtained by a Gaussian convolution (FWHM = 250 cm^{-1}) of the vibronic transitions (sticks) betwen the S_0 and S_1 electronic states.

3.2 PBE

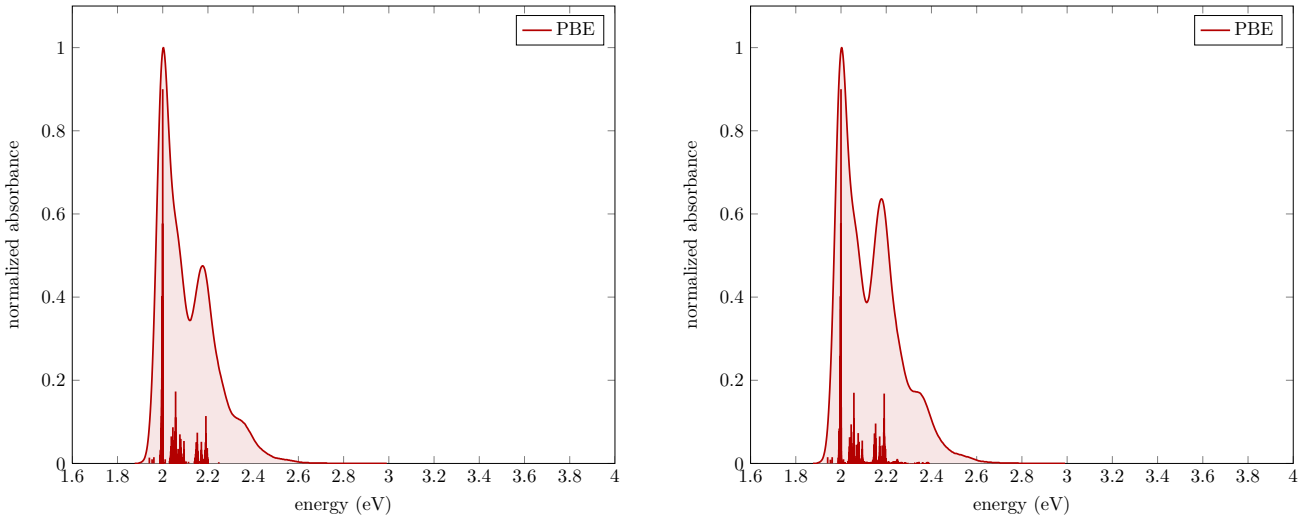

Fig. S23 UV/vis absorption spectra of DAOTA computed within the (left) Franck-Condon and (right) Franck-Condon-Herzberg-Teller approximations at PBE/6-31+G* level of theory in acetonitrile solvent. The envelope of each spectrum is obtained by a Gaussian convolution (FWHM = 250 cm^{-1}) of the vibronic transitions (sticks) betwen the S_0 and S_1 electronic states.

3.3 B3LYP

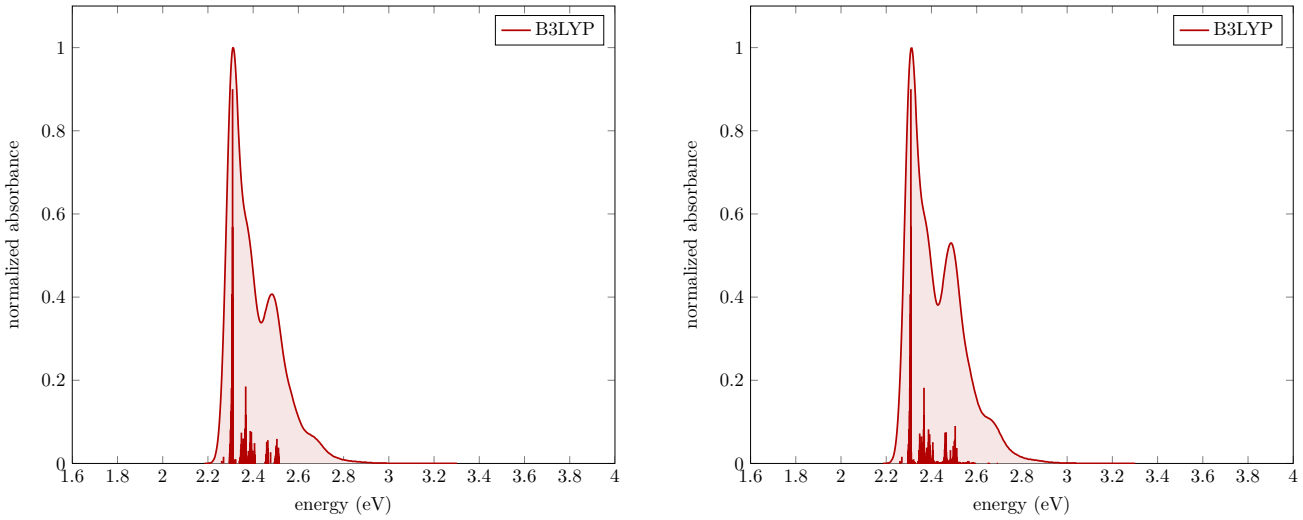

Fig. S24 UV/vis absorption spectra of DAOTA computed within the (left) Franck-Condon and (right) Franck-Condon-Herzberg-Teller approximations at B3LYP/6-31+G* level of theory in acetonitrile solvent. The envelope of each spectrum is obtained by a Gaussian convolution (FWHM = 250 cm^{-1}) of the vibronic transitions (sticks) betwen the S_0 and S_1 electronic states.

3.4 PBE0

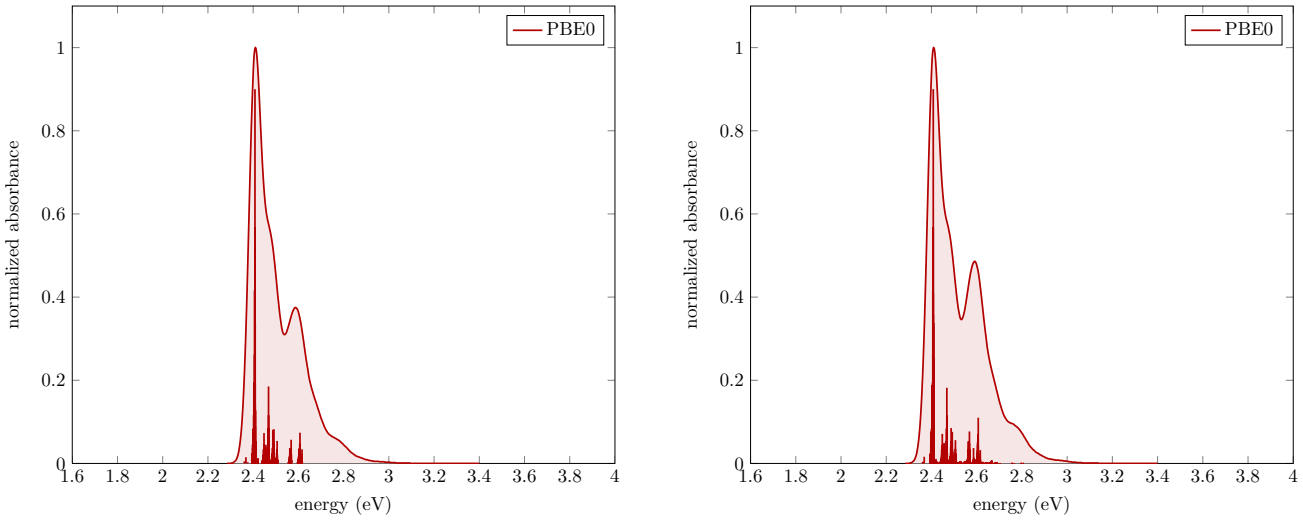

Fig. S25 UV/vis absorption spectra of DAOTA computed within the (left) Franck-Condon and (right) Franck-Condon-Herzberg-Teller approximations at PBE0/6-31+G* level of theory in acetonitrile solvent. The envelope of each spectrum is obtained by a Gaussian convolution (FWHM = 250 cm^{-1}) of the vibronic transitions (sticks) betwen the S_0 and S_1 electronic states.

3.5 M06

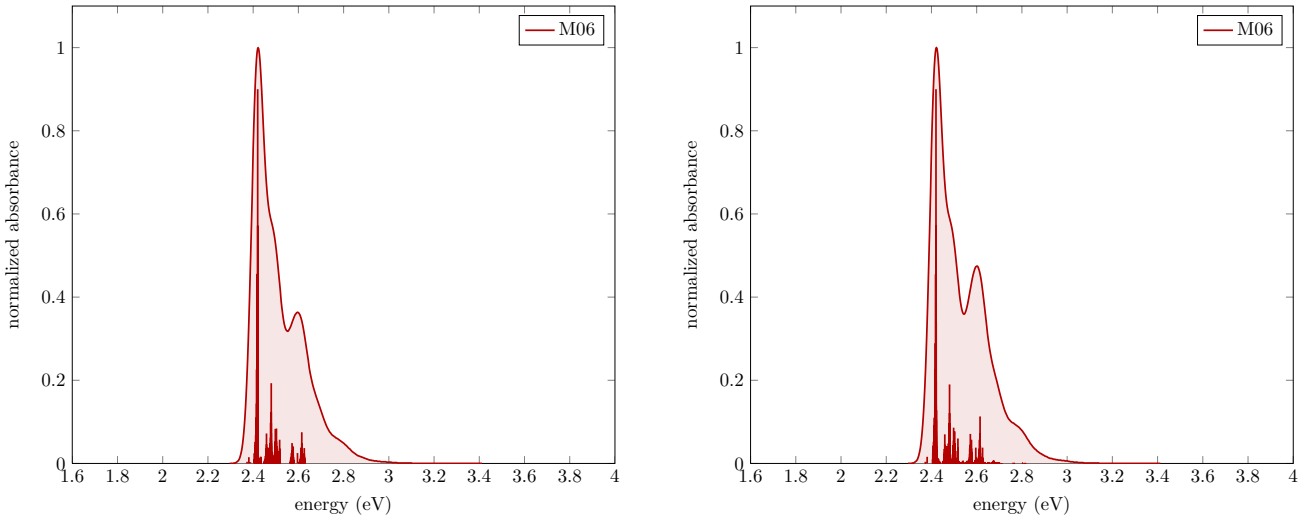

Fig. S26 UV/vis absorption spectra of DAOTA computed within the (left) Franck-Condon and (right) Franck-Condon-Herzberg-Teller approximations at M06/6-31+G* level of theory in acetonitrile solvent. The envelope of each spectrum is obtained by a Gaussian convolution (FWHM = 250 cm^{-1}) of the vibronic transitions (sticks) betwen the S_0 and S_1 electronic states.

3.6 BMK

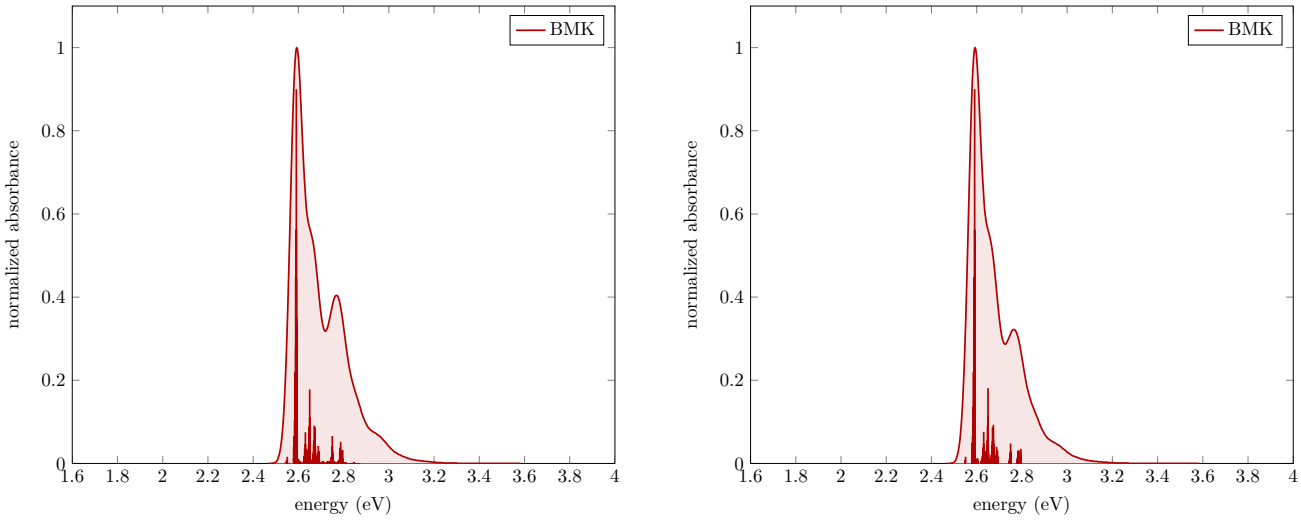

Fig. S27 UV/vis absorption spectra of DAOTA computed within the (left) Franck-Condon and (right) Franck-Condon-Herzberg-Teller approximations at BMK/6-31+G* level of theory in acetonitrile solvent. The envelope of each spectrum is obtained by a Gaussian convolution (FWHM = 250 cm^{-1}) of the vibronic transitions (sticks) betwen the S_0 and S_1 electronic states.

3.7 M06-2X

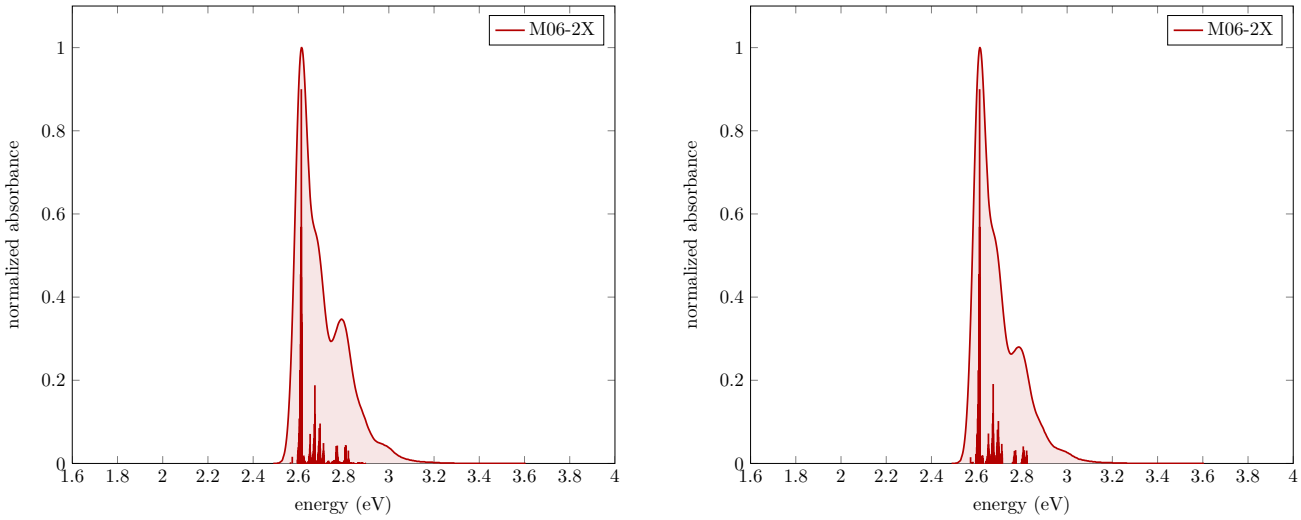

Fig. S28 UV/vis absorption spectra of DAOTA computed within the (left) Franck-Condon and (right) Franck-Condon-Herzberg-Teller approximations at M06-2X/6-31+G* level of theory in acetonitrile solvent. The envelope of each spectrum is obtained by a Gaussian convolution (FWHM = 250 cm^{-1}) of the vibronic transitions (sticks) betwen the S_0 and S_1 electronic states.

3.8 M06-HF

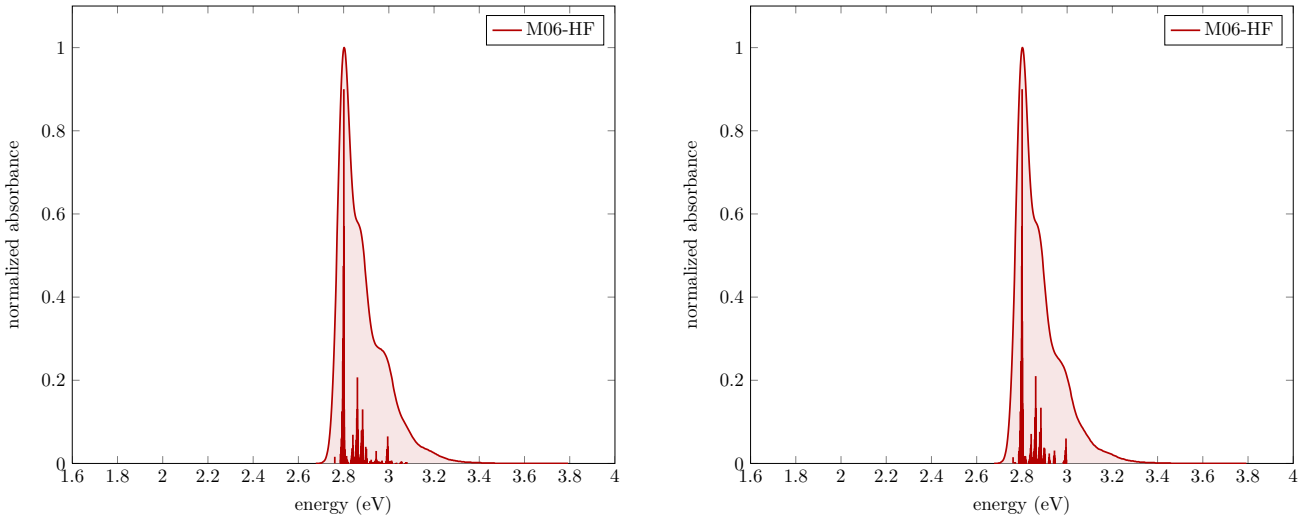

Fig. S29 UV/vis absorption spectra of DAOTA computed within the (left) Franck-Condon and (right) Franck-Condon-Herzberg-Teller approximations at M06-HF/6-31+G* level of theory in acetonitrile solvent. The envelope of each spectrum is obtained by a Gaussian convolution (FWHM = 250 cm^{-1}) of the vibronic transitions (sticks) betwen the S_0 and S_1 electronic states.

3.9 ωB97XD

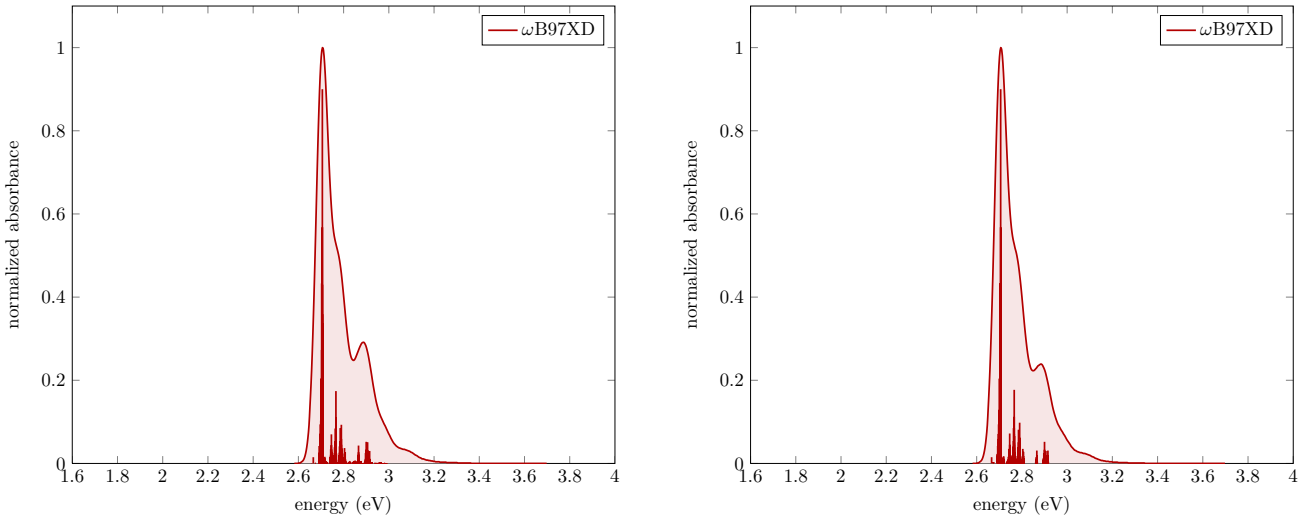

Fig. S30 UV/vis absorption spectra of DAOTA computed within the (left) Franck-Condon and (right) Franck-Condon-Herzberg-Teller approximations at ωB97XD/6-31+G* level of theory in acetonitrile solvent. The envelope of each spectrum is obtained by a Gaussian convolution (FWHM = 250 cm^{-1}) of the vibronic transitions (sticks) betwen the S_0 and S_1 electronic states.

3.10 CAM-B3LYP

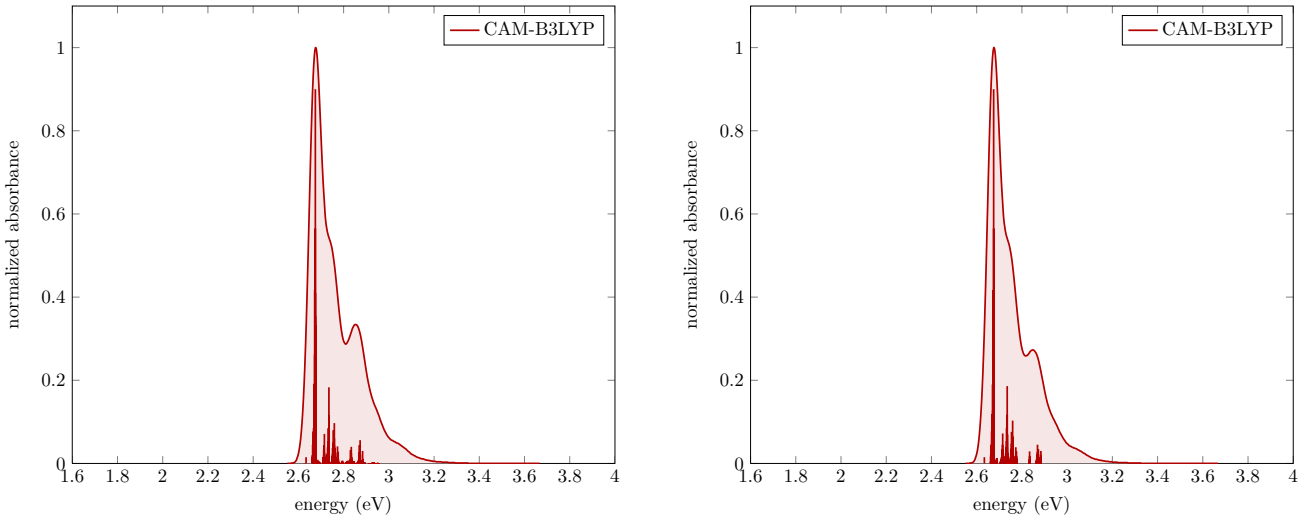

Fig. S31 UV/vis absorption spectra of DAOTA computed within the (left) Franck-Condon and (right) Franck-Condon-Herzberg-Teller approximations at CAM-B3LYP/6-31+G* level of theory in acetonitrile solvent. The envelope of each spectrum is obtained by a Gaussian convolution (FWHM = 250 cm^{-1}) of the vibronic transitions (sticks) betwen the S_0 and S_1 electronic states.

4 TOTA

4.1 SVWN5

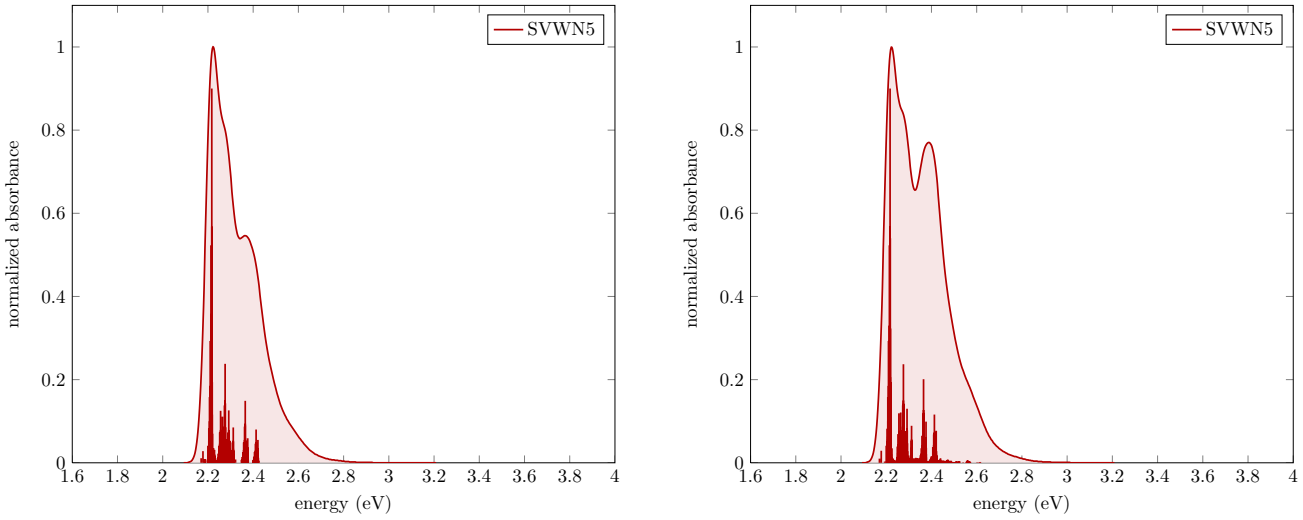

Fig. S32 UV/vis absorption spectra of TOTA computed within the (left) Franck-Condon and (right) Franck-Condon-Herzberg-Teller approximations at SVWN5/6-31+G* level of theory in acetonitrile solvent. The envelope of each spectrum is obtained by a Gaussian convolution (FWHM = 250 cm^{-1}) of the vibronic transitions (sticks) betwen the S_0 and S_1 electronic states.

4.2 PBE

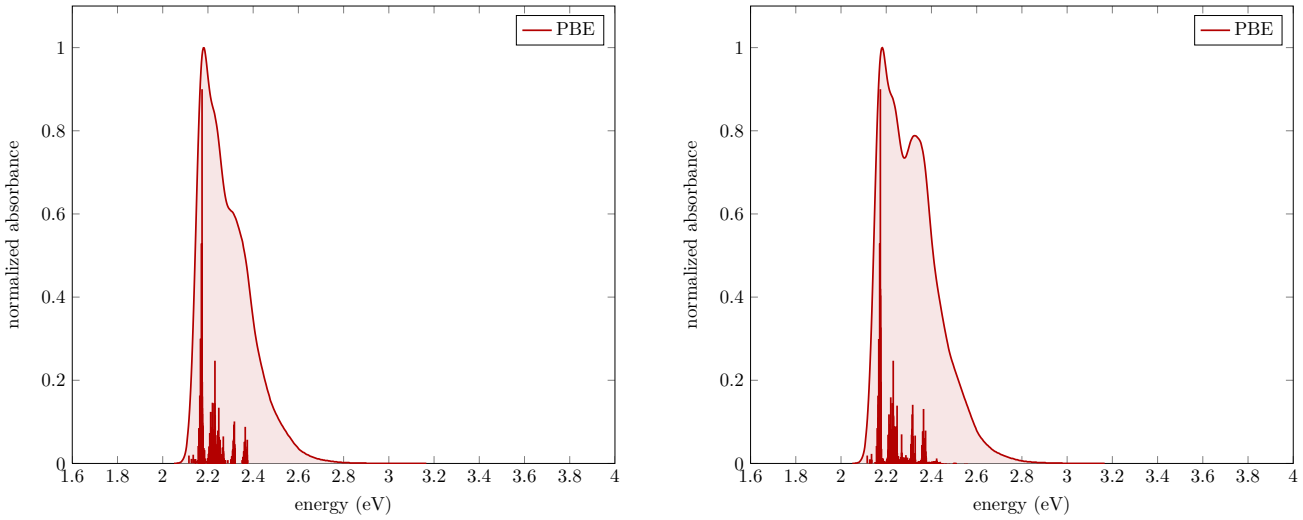

Fig. S33 UV/vis absorption spectra of TOTA computed within the (left) Franck-Condon and (right) Franck-Condon-Herzberg-Teller approximations at PBE/6-31+G* level of theory in acetonitrile solvent. The envelope of each spectrum is obtained by a Gaussian convolution (FWHM = 250 cm^{-1}) of the vibronic transitions (sticks) betwen the S_0 and S_1 electronic states.

4.3 B3LYP

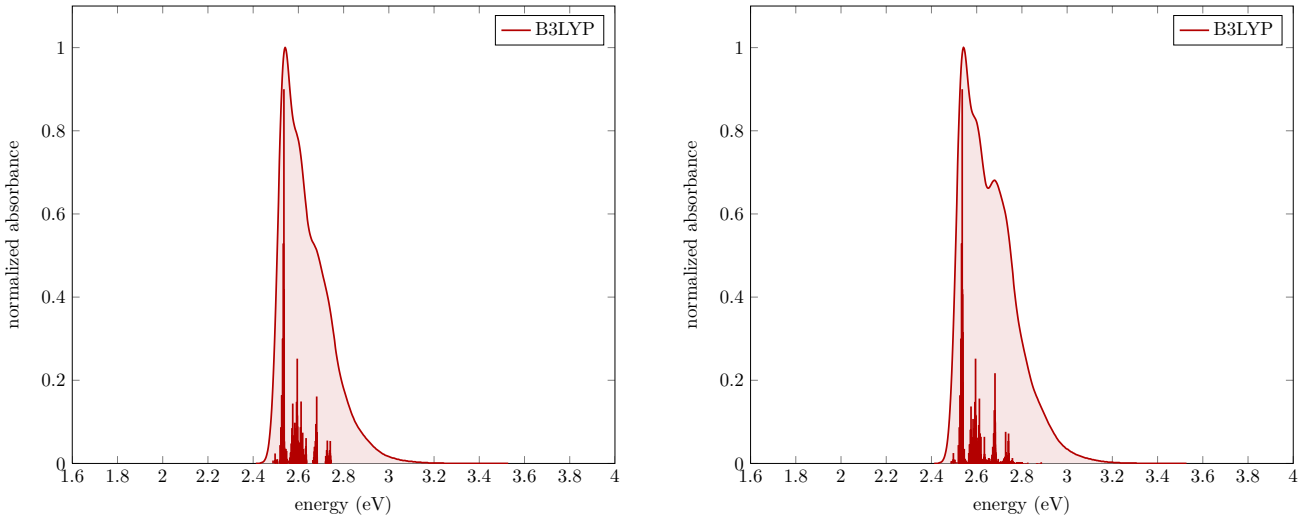

Fig. S34 UV/vis absorption spectra of TOTA computed within the (left) Franck-Condon and (right) Franck-Condon-Herzberg-Teller approximations at B3LYP/6-31+G* level of theory in acetonitrile solvent. The envelope of each spectrum is obtained by a Gaussian convolution (FWHM = 250 cm^{-1}) of the vibronic transitions (sticks) betwen the S_0 and S_1 electronic states.

4.4 PBE0

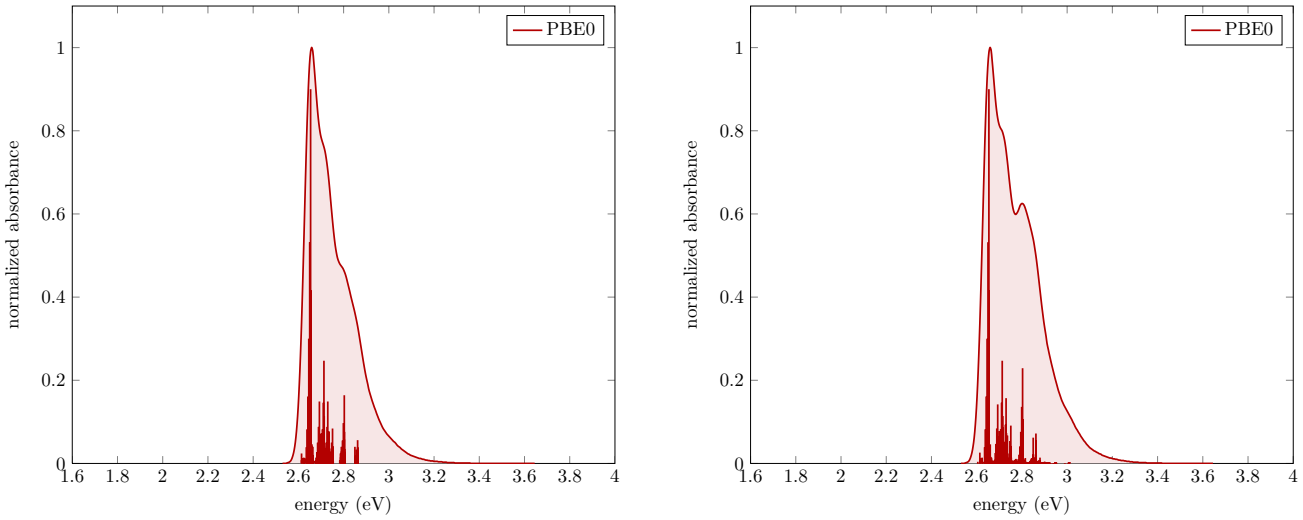

Fig. S35 UV/vis absorption spectra of TOTA computed within the (left) Franck-Condon and (right) Franck-Condon-Herzberg-Teller approximations at PBE0/6-31+G* level of theory in acetonitrile solvent. The envelope of each spectrum is obtained by a Gaussian convolution (FWHM = 250 cm^{-1}) of the vibronic transitions (sticks) betwen the S_0 and S_1 electronic states.

4.5 M06

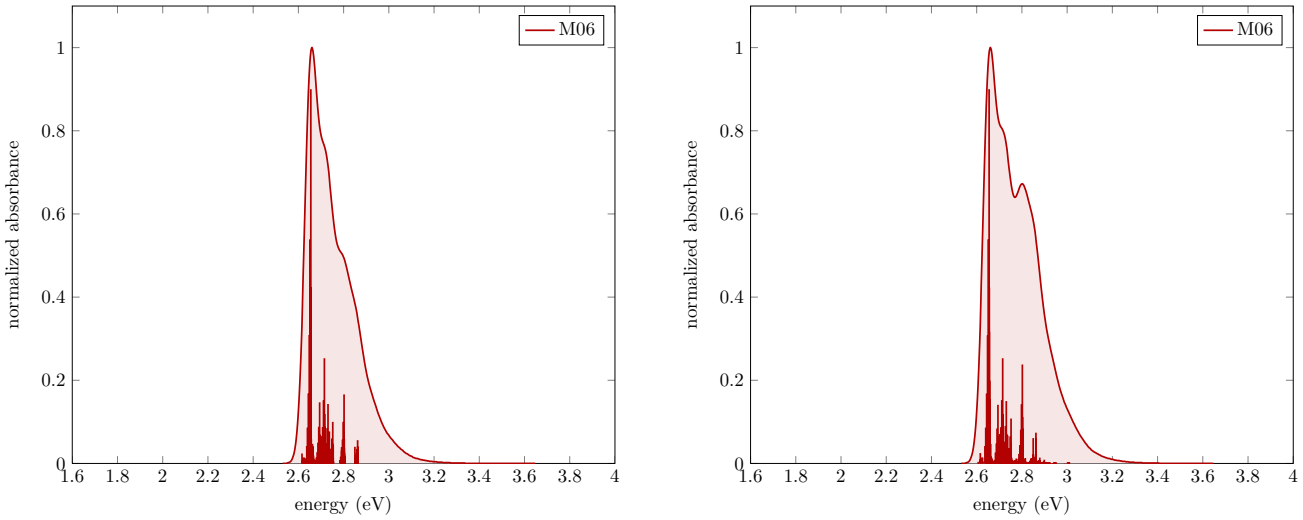

Fig. S36 UV/vis absorption spectra of TOTA computed within the (left) Franck-Condon and (right) Franck-Condon-Herzberg-Teller approximations at M06/6-31+G* level of theory in acetonitrile solvent. The envelope of each spectrum is obtained by a Gaussian convolution (FWHM = 250 cm^{-1}) of the vibronic transitions (sticks) betwen the S_0 and S_1 electronic states.

4.6 BMK

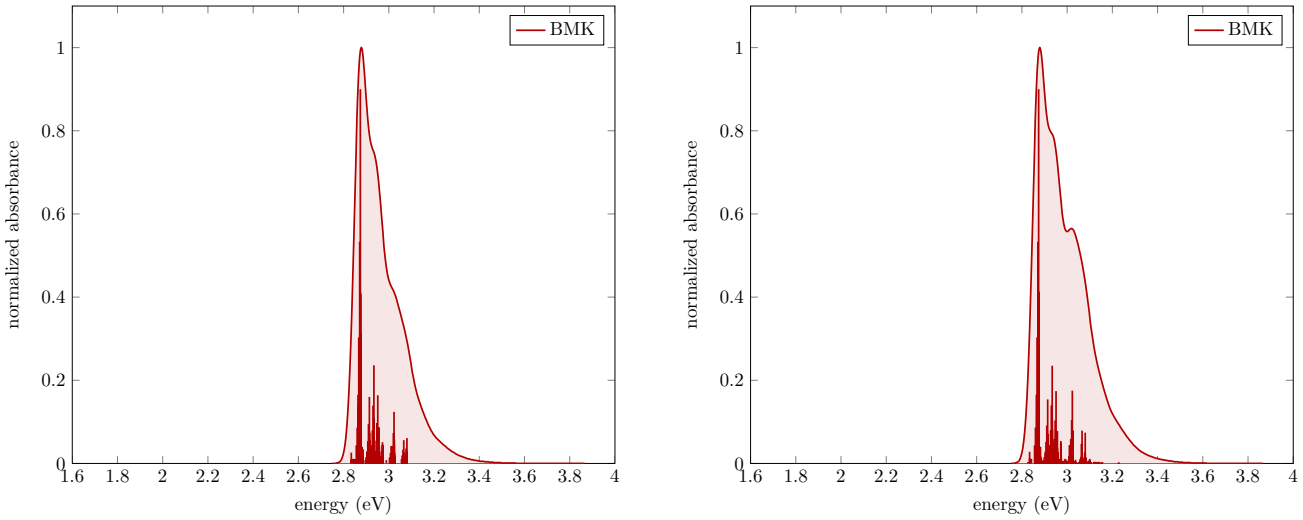

Fig. S37 UV/vis absorption spectra of TOTA computed within the (left) Franck-Condon and (right) Franck-Condon-Herzberg-Teller approximations at BMK/6-31+G* level of theory in acetonitrile solvent. The envelope of each spectrum is obtained by a Gaussian convolution (FWHM = 250 cm^{-1}) of the vibronic transitions (sticks) betwen the S_0 and S_1 electronic states.

4.7 M06-2X

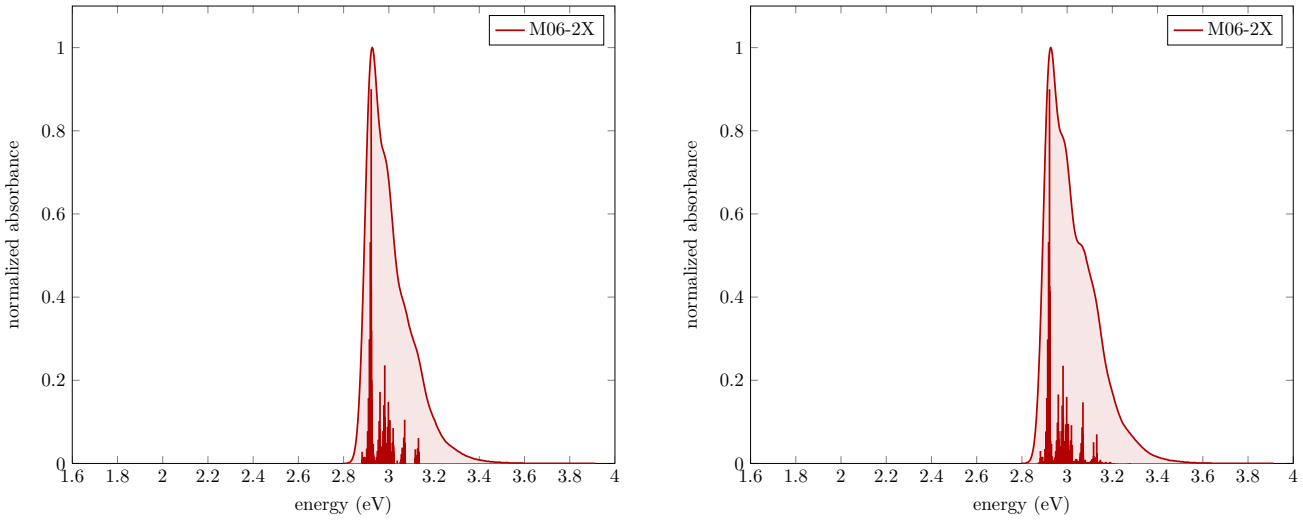

Fig. S38 UV/vis absorption spectra of TOTA computed within the (left) Franck-Condon and (right) Franck-Condon-Herzberg-Teller approximations at M06-2X/6-31+G* level of theory in acetonitrile solvent. The envelope of each spectrum is obtained by a Gaussian convolution (FWHM = 250 cm^{-1}) of the vibronic transitions (sticks) betwen the S_0 and S_1 electronic states.

4.8 M06-HF

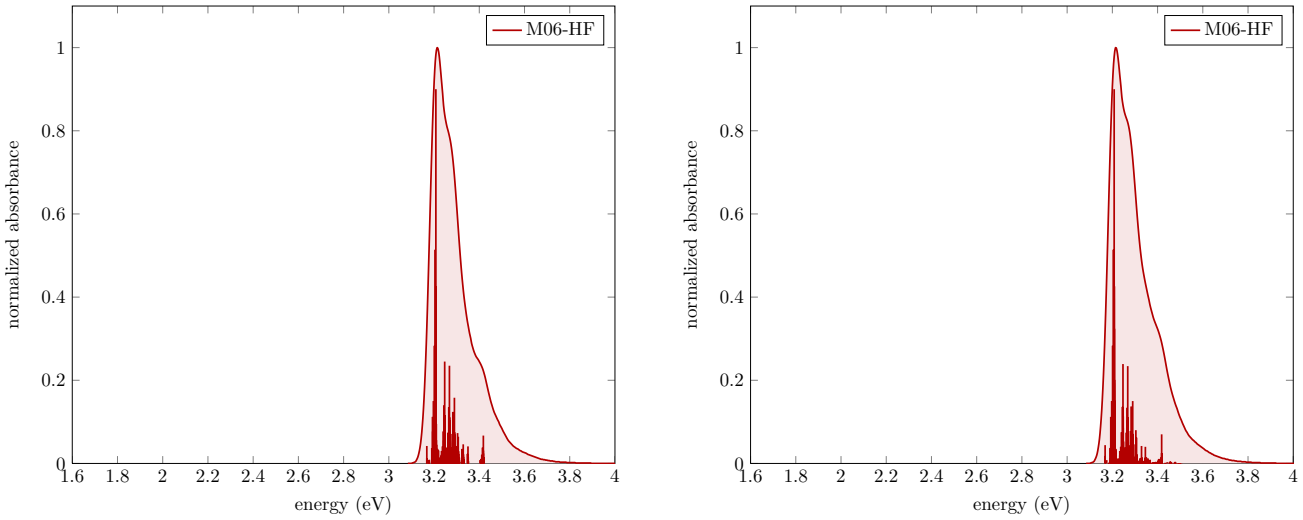

Fig. S39 UV/vis absorption spectra of TOTA computed within the (left) Franck-Condon and (right) Franck-Condon-Herzberg-Teller approximations at M06-HF/6-31+G* level of theory in acetonitrile solvent. The envelope of each spectrum is obtained by a Gaussian convolution (FWHM = 250 cm^{-1}) of the vibronic transitions (sticks) betwen the S_0 and S_1 electronic states.

4.9 ωB97XD

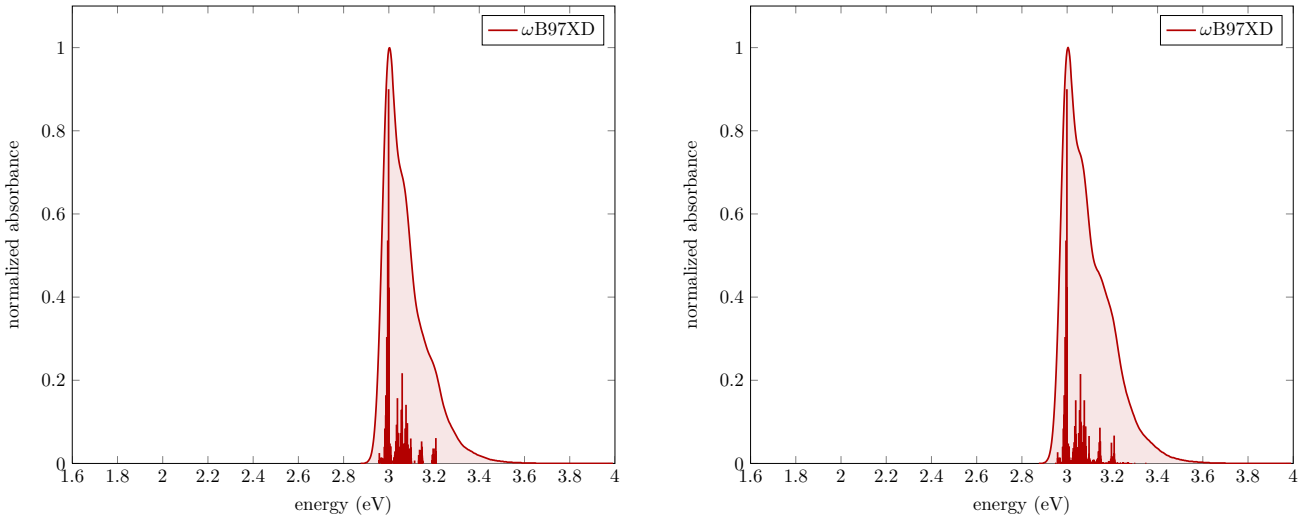

Fig. S40 UV/vis absorption spectra of TOTA computed within the (left) Franck-Condon and (right) Franck-Condon-Herzberg-Teller approximations at ωB97XD/6-31+G* level of theory in acetonitrile solvent. The envelope of each spectrum is obtained by a Gaussian convolution (FWHM = 250 cm^{-1}) of the vibronic transitions (sticks) betwen the S_0 and S_1 electronic states.

4.10 CAM-B3LYP

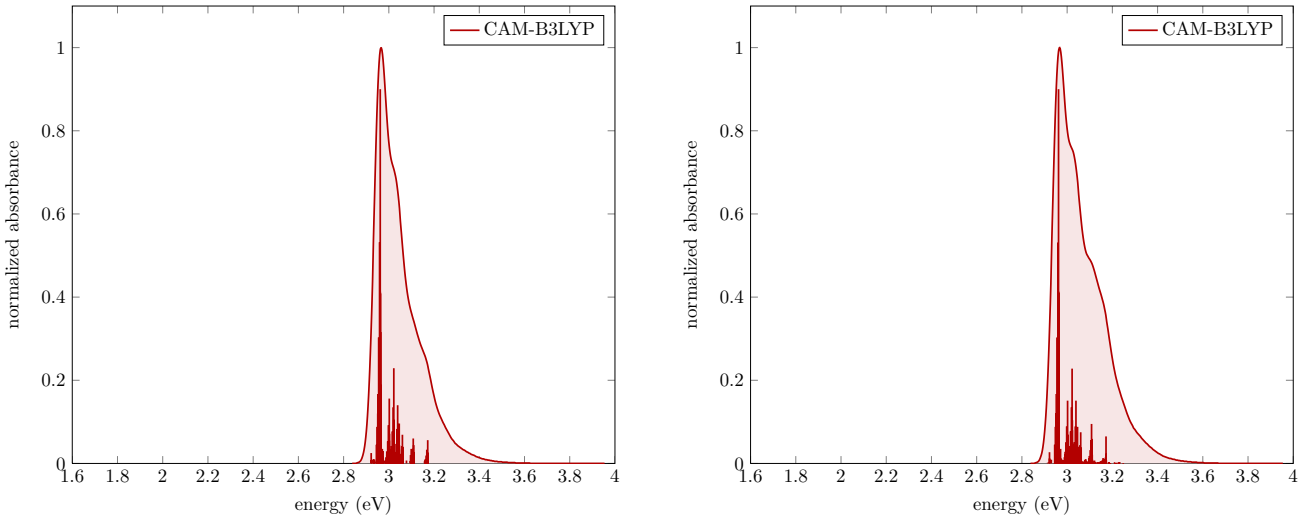

Fig. S41 UV/vis absorption spectra of TOTA computed within the (left) Franck-Condon and (right) Franck-Condon-Herzberg-Teller approximations at CAM-B3LYP/6-31+G* level of theory in acetonitrile solvent. The envelope of each spectrum is obtained by a Gaussian convolution (FWHM = 250 cm^{-1}) of the vibronic transitions (sticks) betwen the S_0 and S_1 electronic states.

Part II

Basis-Set Benchmark

5 TATA

5.1 STO-3G

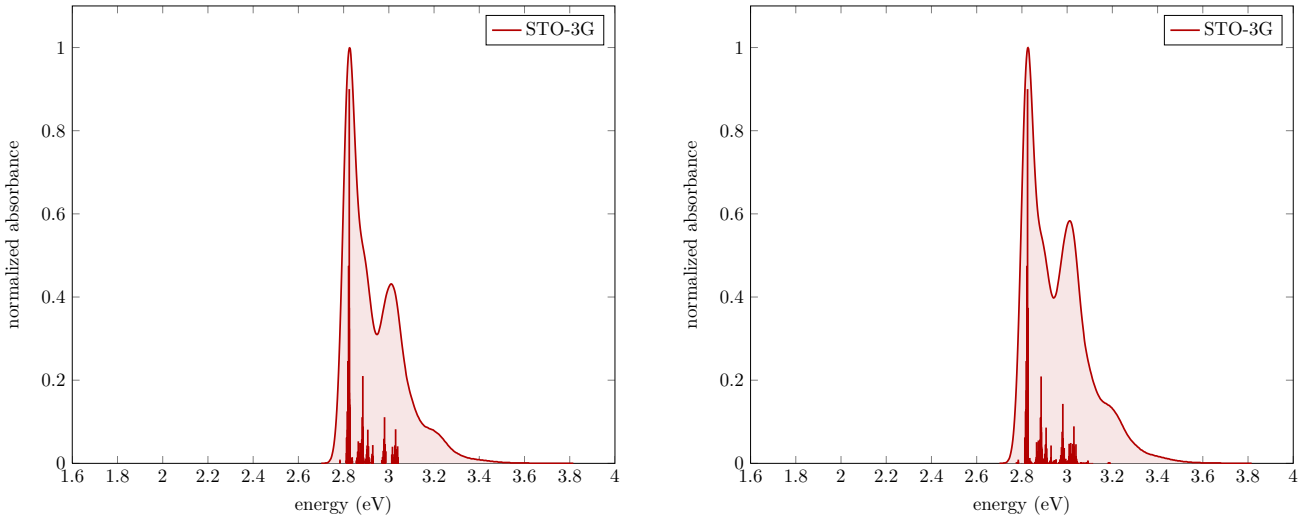

Fig. S42 UV/vis absorption spectra of TATA computed within the (left) Franck-Condon and (right) Franck-Condon-Herzberg-Teller approximations at PBE0/STO-3G level of theory in acetonitrile solvent. The envelope of each spectrum is obtained by a Gaussian convolution (FWHM = 250 cm^{-1}) of the vibronic transitions (sticks) betwen the S_0 and S_1 electronic states.

5.2 6-31G

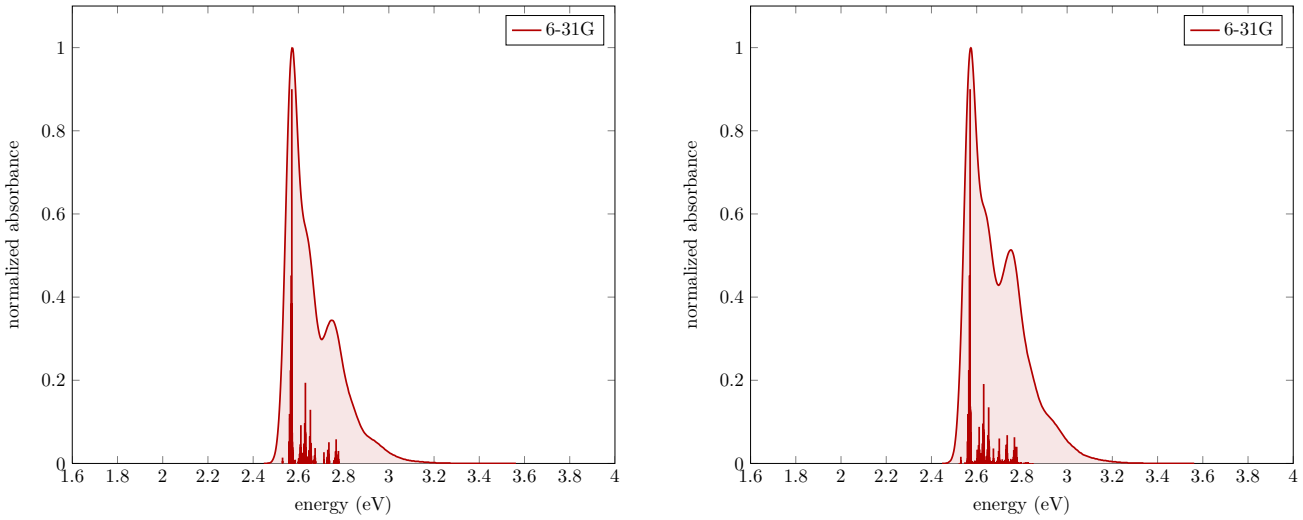

Fig. S43 UV/vis absorption spectra of TATA computed within the (left) Franck-Condon and (right) Franck-Condon-Herzberg-Teller approximations at PBE0/6-31G level of theory in acetonitrile solvent. The envelope of each spectrum is obtained by a Gaussian convolution (FWHM = 250 cm^{-1}) of the vibronic transitions (sticks) betwen the S_0 and S_1 electronic states.

5.3 6-31+G*

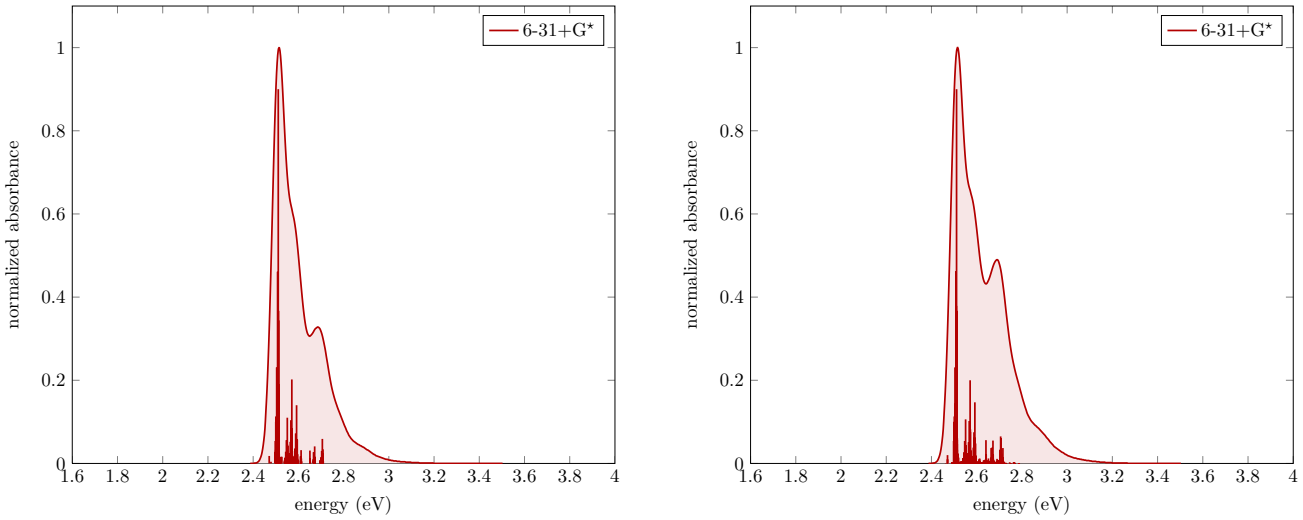

Fig. S44 UV/vis absorption spectra of TATA computed within the (left) Franck-Condon and (right) Franck-Condon-Herzberg-Teller approximations at PBE0/6-31+G* level of theory in acetonitrile solvent. The envelope of each spectrum is obtained by a Gaussian convolution (FWHM = 250 cm^{-1}) of the vibronic transitions (sticks) betwen the S_0 and S_1 electronic states.

5.4 6-31++G**

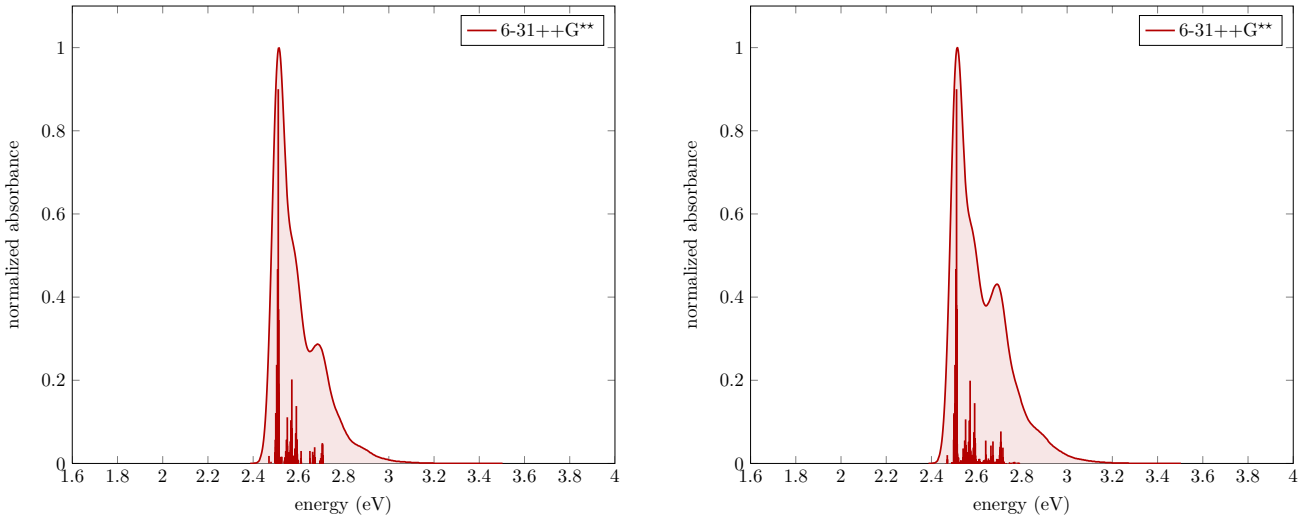

Fig. S45 UV/vis absorption spectra of TATA computed within the (left) Franck-Condon and (right) Franck-Condon-Herzberg-Teller approximations at PBE0/6-31++G** level of theory in acetonitrile solvent. The envelope of each spectrum is obtained by a Gaussian convolution (FWHM = 250 cm^{-1}) of the vibronic transitions (sticks) betwen the S_0 and S_1 electronic states.

5.5 6-311G

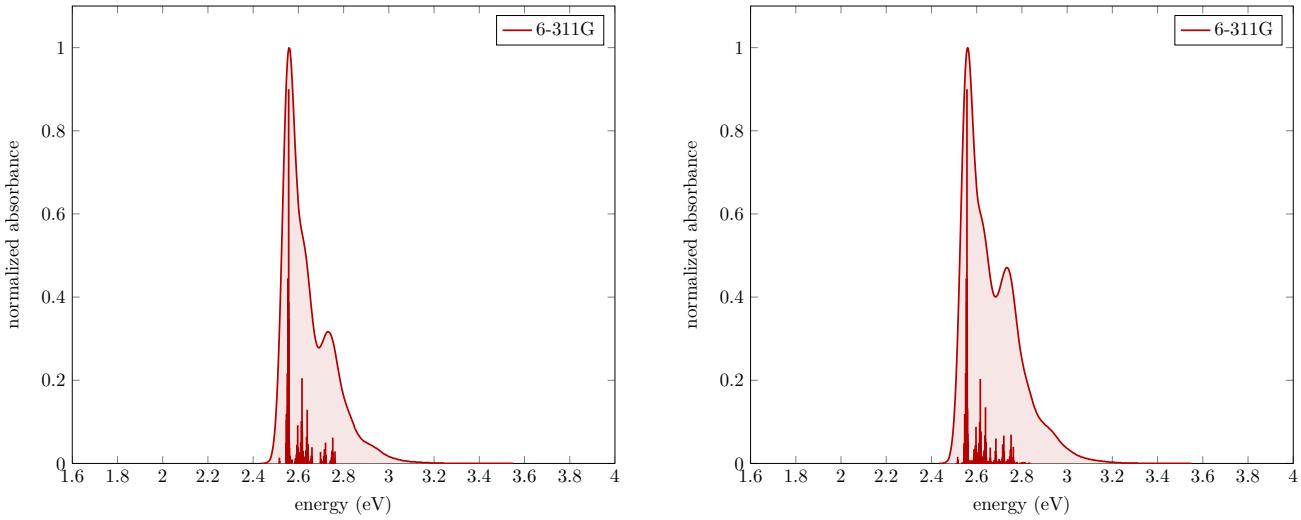

Fig. S46 UV/vis absorption spectra of TATA computed within the (left) Franck-Condon and (right) Franck-Condon-Herzberg-Teller approximations at PBE0/6-311G level of theory in acetonitrile solvent. The envelope of each spectrum is obtained by a Gaussian convolution (FWHM = 250 cm^{-1}) of the vibronic transitions (sticks) betwen the S_0 and S_1 electronic states.

5.6 6-311+G*

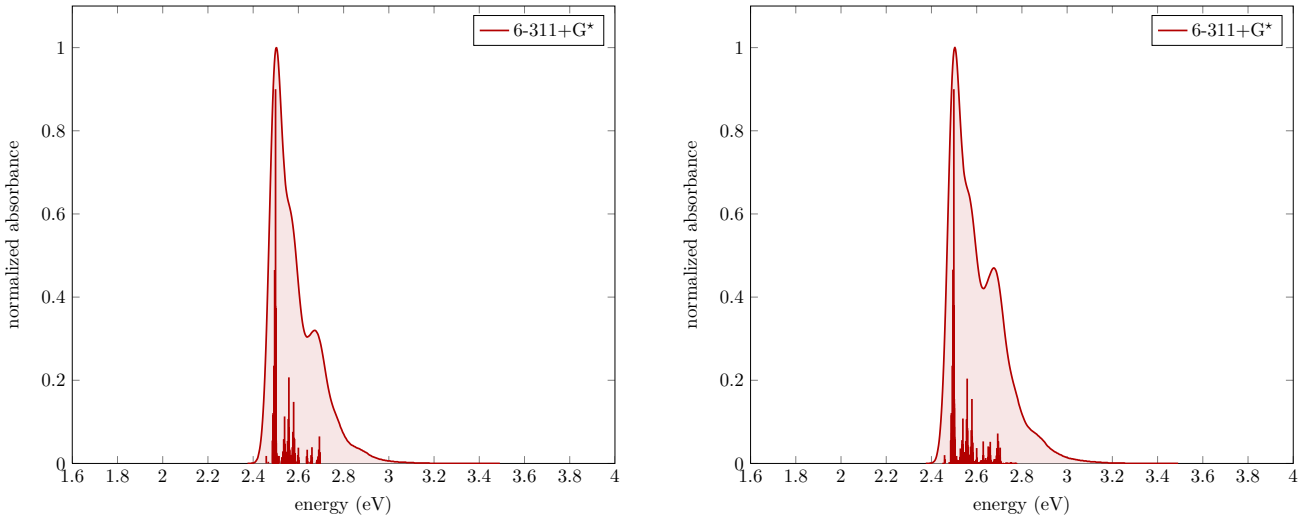

Fig. S47 UV/vis absorption spectra of TATA computed within the (left) Franck-Condon and (right) Franck-Condon-Herzberg-Teller approximations at PBE0/6-311+G* level of theory in acetonitrile solvent. The envelope of each spectrum is obtained by a Gaussian convolution (FWHM = 250 cm^{-1}) of the vibronic transitions (sticks) betwen the S_0 and S_1 electronic states.

5.7 6-311++G**

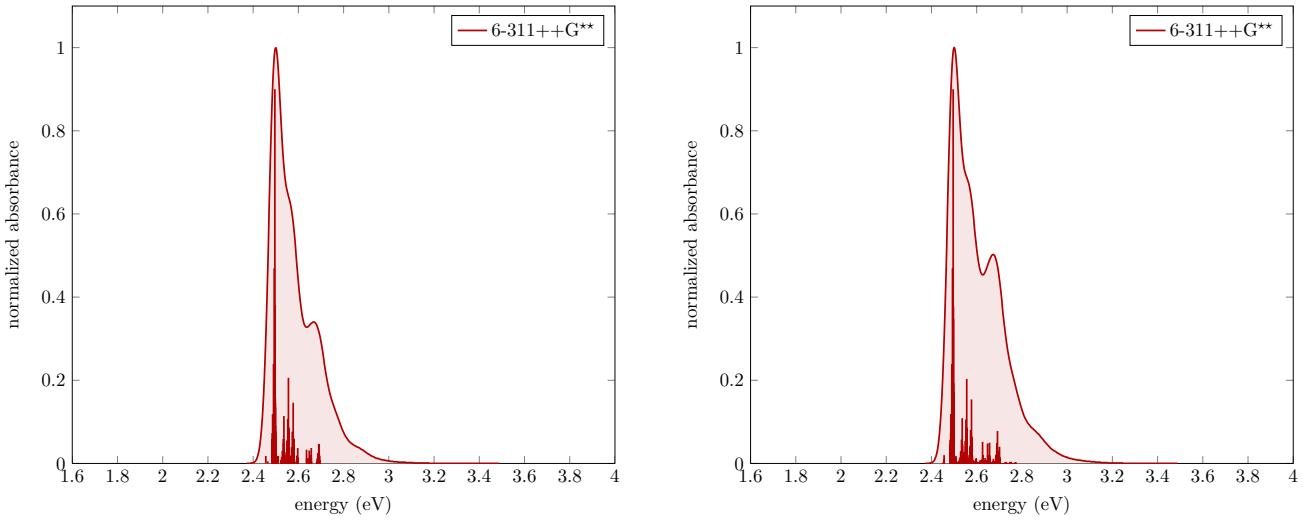

Fig. S48 UV/vis absorption spectra of TATA computed within the (left) Franck-Condon and (right) Franck-Condon-Herzberg-Teller approximations at PBE0/6-311++G** level of theory in acetonitrile solvent. The envelope of each spectrum is obtained by a Gaussian convolution (FWHM = 250 cm^{-1}) of the vibronic transitions (sticks) betwen the S_0 and S_1 electronic states.

5.8 6-311++G($3df$,$3pd$)

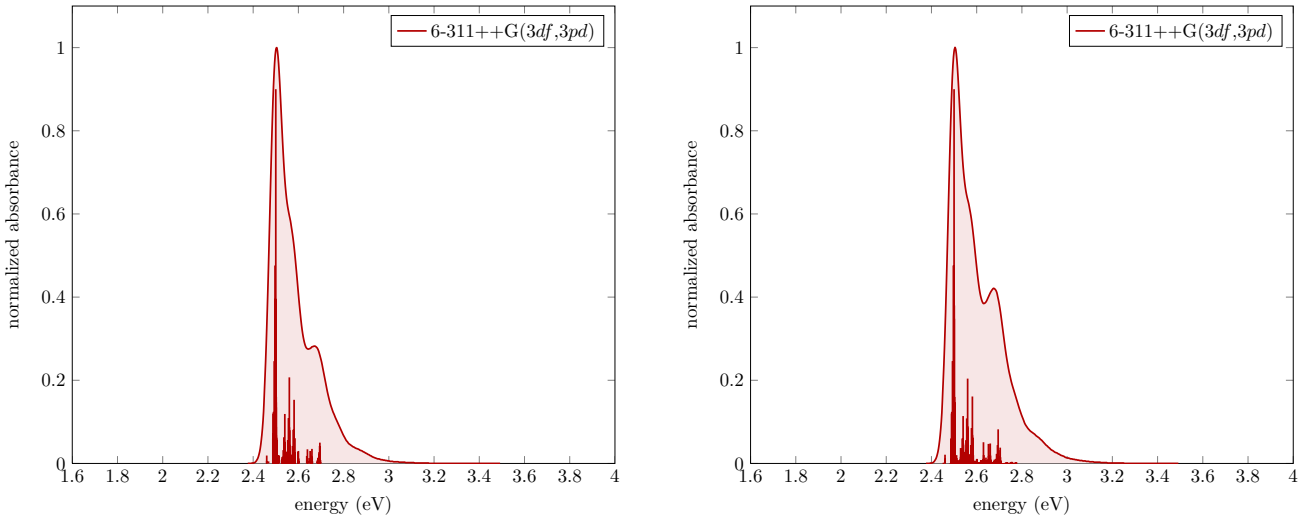

Fig. S49 UV/vis absorption spectra of TATA computed within the (left) Franck-Condon and (right) Franck-Condon-Herzberg-Teller approximations at PBE0/6-311++G($3df$,$3pd$) level of theory in acetonitrile solvent. The envelope of each spectrum is obtained by a Gaussian convolution (FWHM = 250 cm^{-1}) of the vibronic transitions (sticks) betwen the S_0 and S_1 electronic states.

Part III

Solvent Benchmark

6 TATA

6.1 gaz

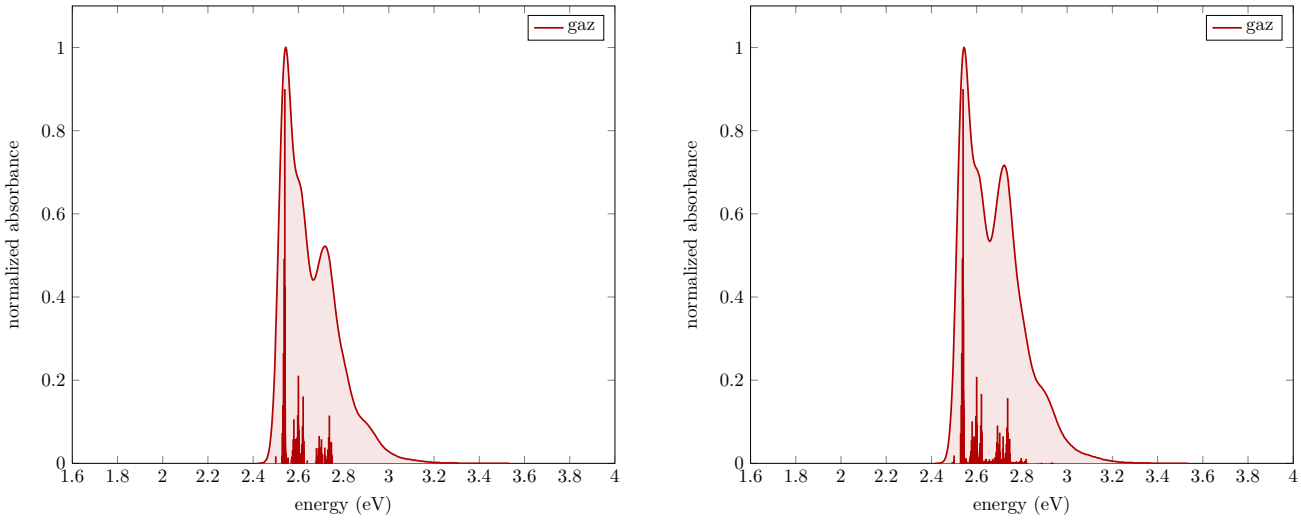

Fig. S50 UV/vis absorption spectra of TATA computed within the (left) Franck-Condon and (right) Franck-Condon-Herzberg-Teller approximations at PBE0/6-31+G* level of theory in gaz solvent. The envelope of each spectrum is obtained by a Gaussian convolution (FWHM = 250 cm^{-1}) of the vibronic transitions (sticks) betwen the S_0 and S_1 electronic states.

6.2 *n*-octane

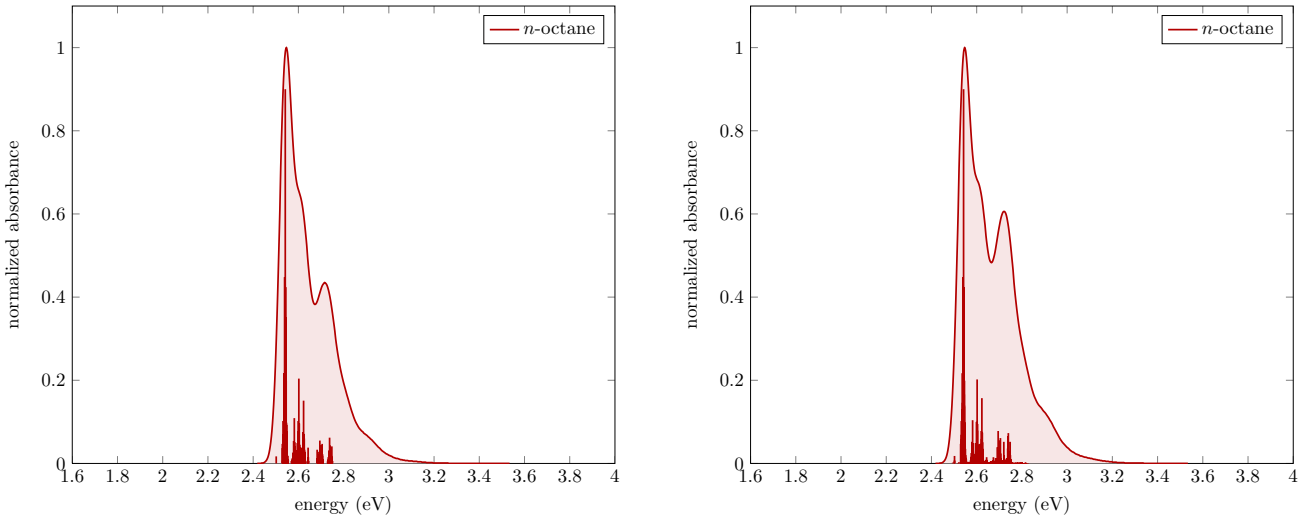

Fig. S51 UV/vis absorption spectra of TATA computed within the (left) Franck-Condon and (right) Franck-Condon-Herzberg-Teller approximations at PBE0/6-31+G* level of theory in *n*-octane solvent. The envelope of each spectrum is obtained by a Gaussian convolution (FWHM = 250 cm^{-1}) of the vibronic transitions (sticks) betwen the S_0 and S_1 electronic states.

6.3 acetonitrile

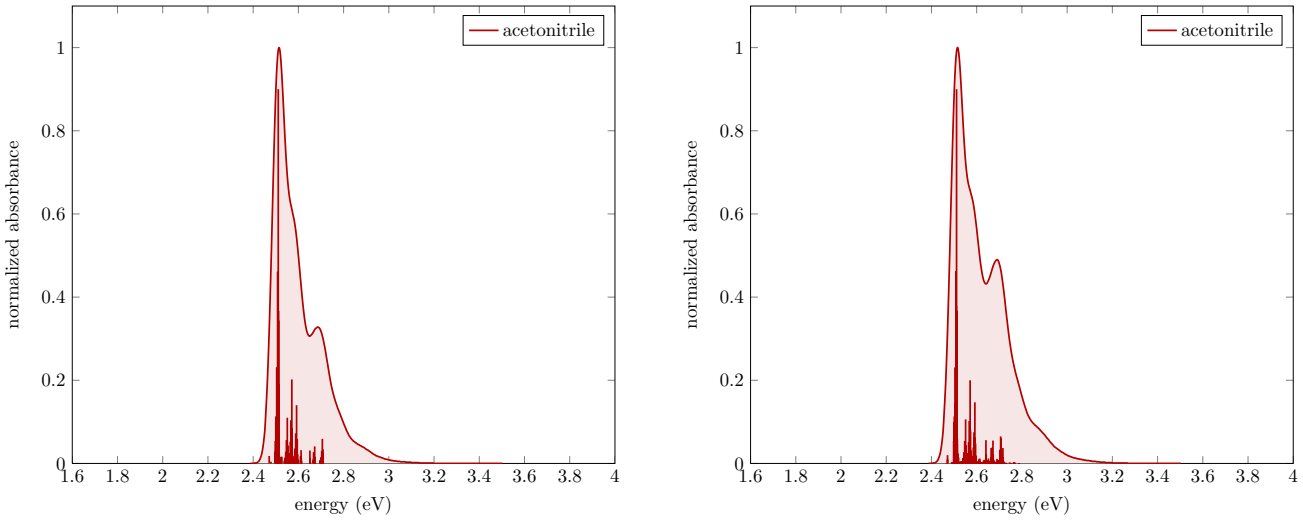

Fig. S52 UV/vis absorption spectra of TATA computed within the (left) Franck-Condon and (right) Franck-Condon-Herzberg-Teller approximations at PBE0/6-31+G* level of theory in acetonitrile solvent. The envelope of each spectrum is obtained by a Gaussian convolution (FWHM = 250 cm^{-1}) of the vibronic transitions (sticks) betwen the S_0 and S_1 electronic states.

6.4 1-hexanol

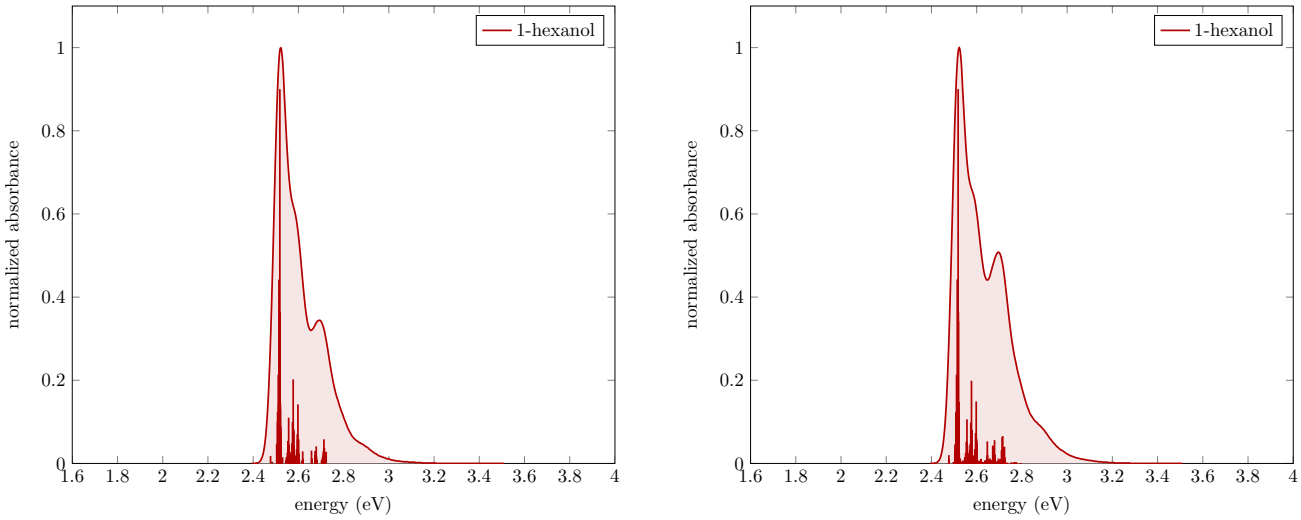

Fig. S53 UV/vis absorption spectra of TATA computed within the (left) Franck-Condon and (right) Franck-Condon-Herzberg-Teller approximations at PBE0/6-31+G* level of theory in 1-hexanol solvent. The envelope of each spectrum is obtained by a Gaussian convolution (FWHM = 250 cm^{-1}) of the vibronic transitions (sticks) betwen the S_0 and S_1 electronic states.

6.5 dimethylsulfoxide

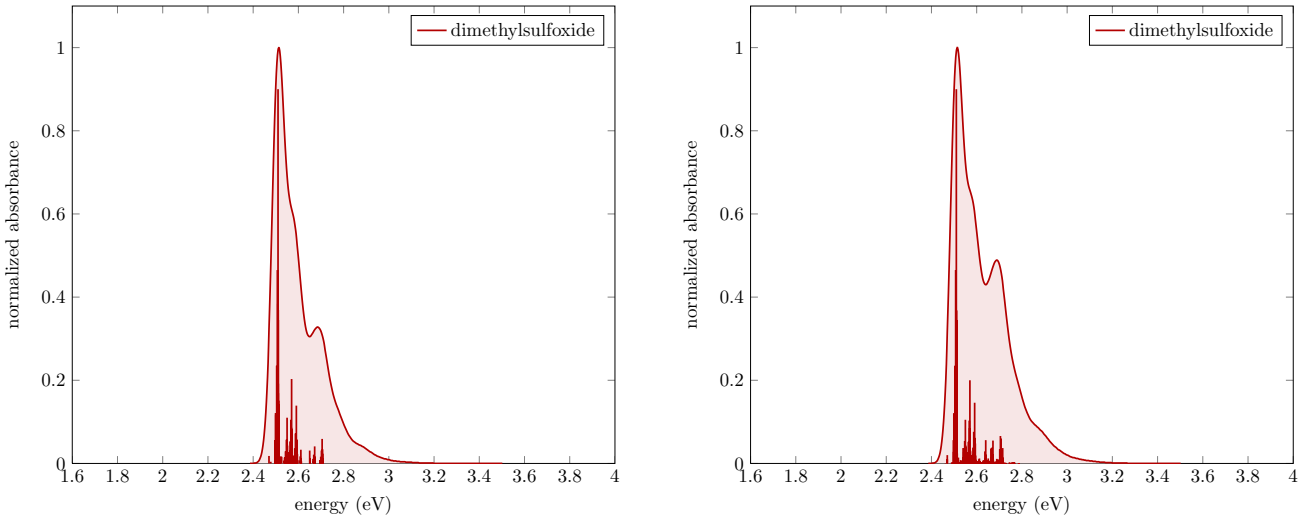

Fig. S54 UV/vis absorption spectra of TATA computed within the (left) Franck-Condon and (right) Franck-Condon-Herzberg-Teller approximations at PBE0/6-31+G* level of theory in dimethylsulfoxide solvent. The envelope of each spectrum is obtained by a Gaussian convolution (FWHM = 250 cm^{-1}) of the vibronic transitions (sticks) betwen the S_0 and S_1 electronic states.

6.6 water

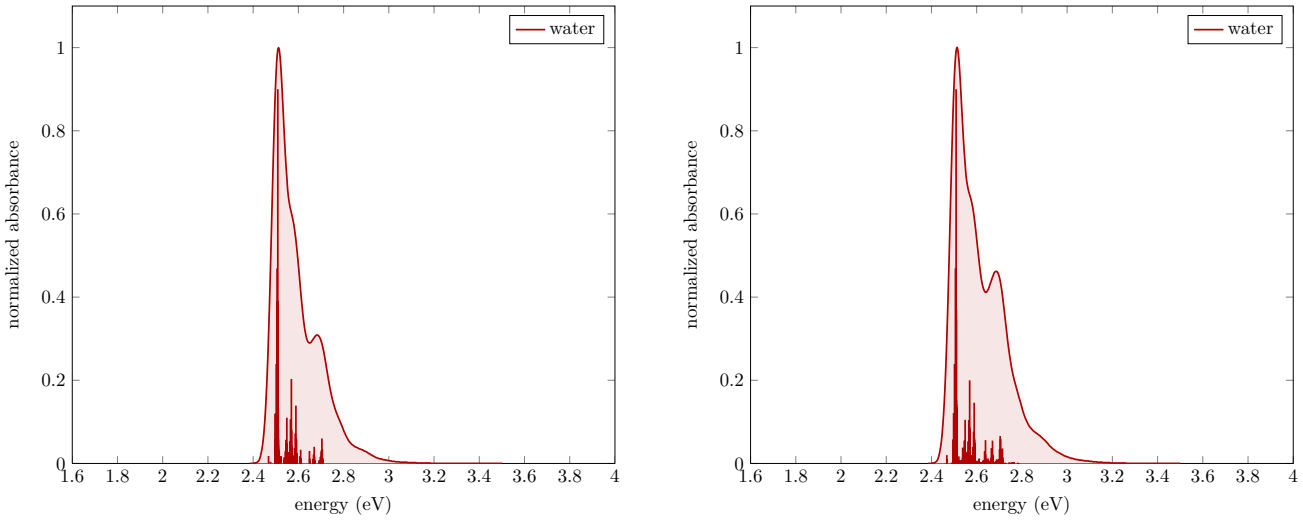

Fig. S55 UV/vis absorption spectra of TATA computed within the (left) Franck-Condon and (right) Franck-Condon-Herzberg-Teller approximations at PBE0/6-31+G* level of theory in water solvent. The envelope of each spectrum is obtained by a Gaussian convolution (FWHM = 250 cm^{-1}) of the vibronic transitions (sticks) betwen the S_0 and S_1 electronic states.