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Supporting information

Solvatochromic shifts of single-walled carbon nanotubes in nonpolar microenvironments

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Deconvolution of the spectra

Figure S1 shows a typical simulated curve (red) compared to the experimental curve (blue) as well as the deconvoluted peaks corresponding to each (*n*,*m*) type. The simulated curve shows a good fit to the experimental curve. The peaks for each (*n*,*m*) component are shown under the simulated curve. Note that the attached solvent characterization sheets show the deconvolution for all PL spectra.

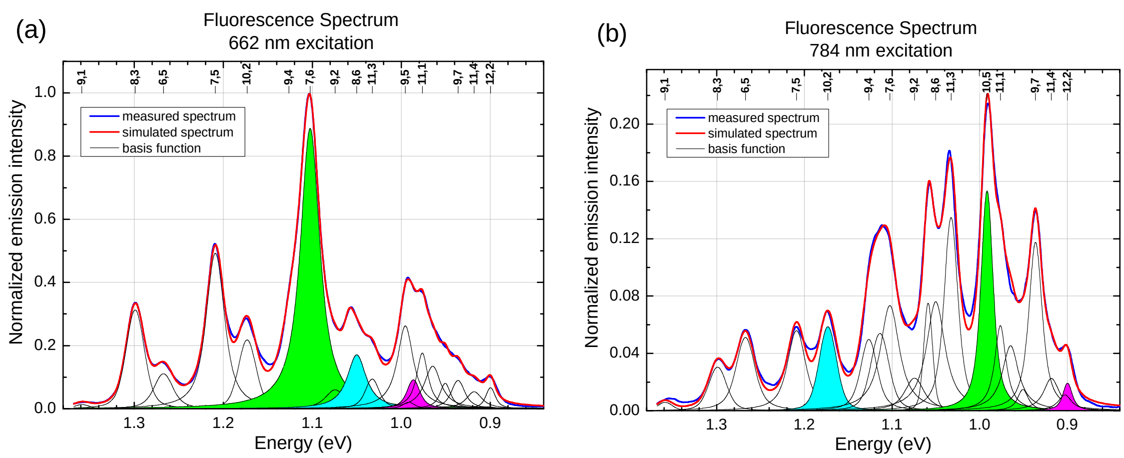
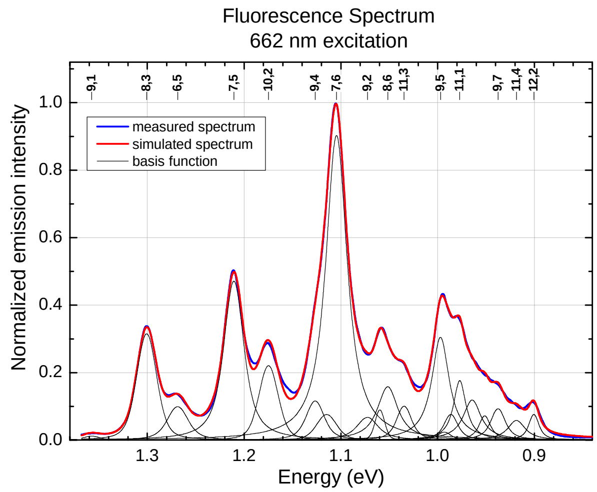


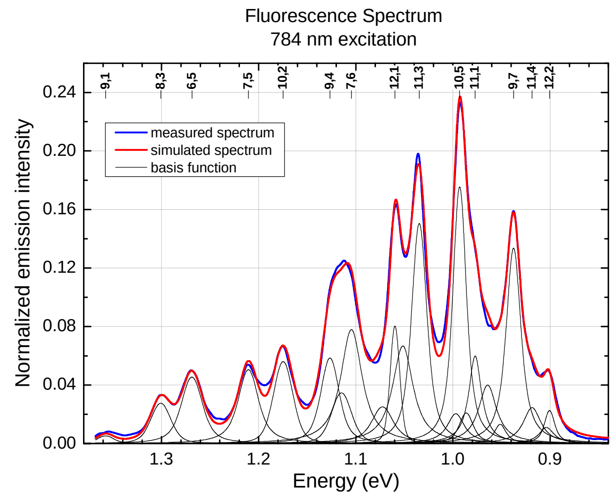
Figure S1: Deconvolution of PL emission spectra for excitation at (a) 662 and (b) 784 nm. Weighting factors were assigned to each peak based on the amount of overlap with other peaks and the intensity. Those peaks highlighted in (a) show examples of the three weighting factors associated with overlap while (b) shows those associated with intensity. The green, blue, and purple curves were assigned values of 1, 0.5, and 0.25, respectively.

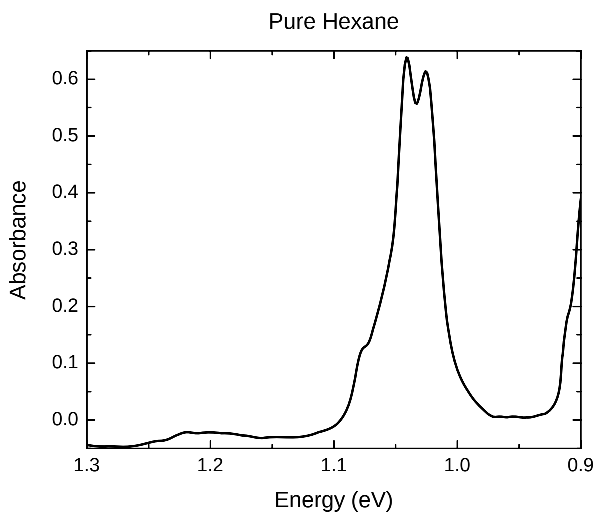
Solvent characterization sheets

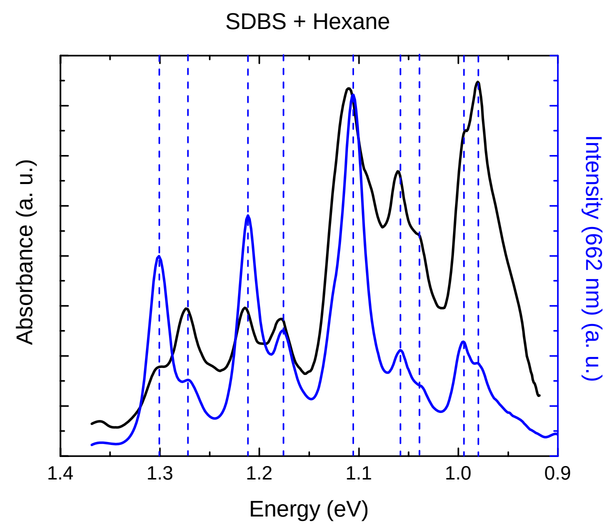
The results of each solvent are summarized in the following sheets for easy reference. These data sheets include the PL emission from excitation at 662 and 784 nm, the absorbance spectrum for the pure solvent, comparison of the absorbance and PL emission spectra, and a table of the peak position and solvatochromic shift of each (*n*,*m*) type.

Hexane (ε = 1.89, η = 1.37, D = 0, $f(\eta^2)$ = 0.369)





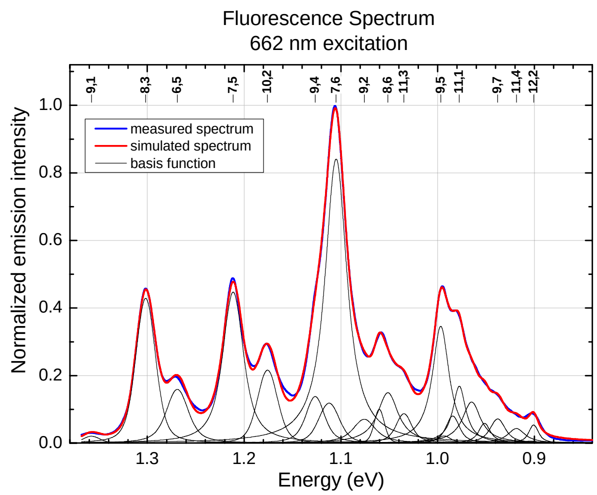


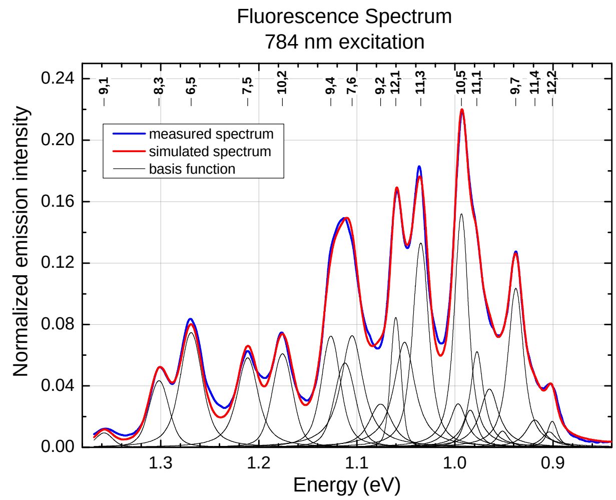


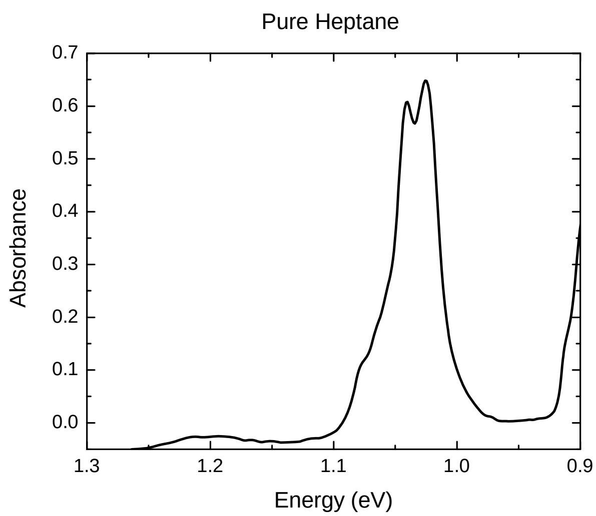
Type	E_{11} (eV)	E_{11} Shift (meV)[a]
(8, 3)	1.301	67
(6, 5)	1.269	83
(7, 5)	1.211	63
(10, 2)	1.175	49
(9, 4)	1.127	44
(7, 6)	1.104	56
(12, 1)	1.060	33
(8, 6)	1.052	48
(11, 3)	1.035	33
(9, 5)	0.997	46
(10, 5)	0.993	31
(11, 1)	0.977	81
(9, 7)	0.938	30
(12, 2)	0.901	50

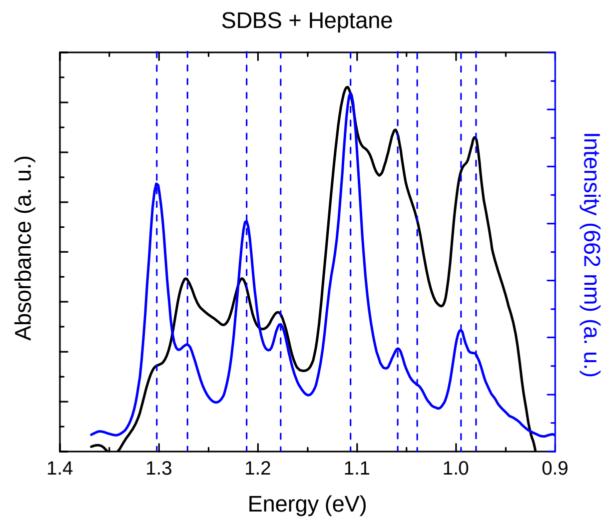
[a] Shift in comparison to fluorescence emission for SWNTs in air

<u>**Heptane**</u> (ε = 1.92, η = 1.39, D = 0, $f(\eta^2)$ = 0.383)





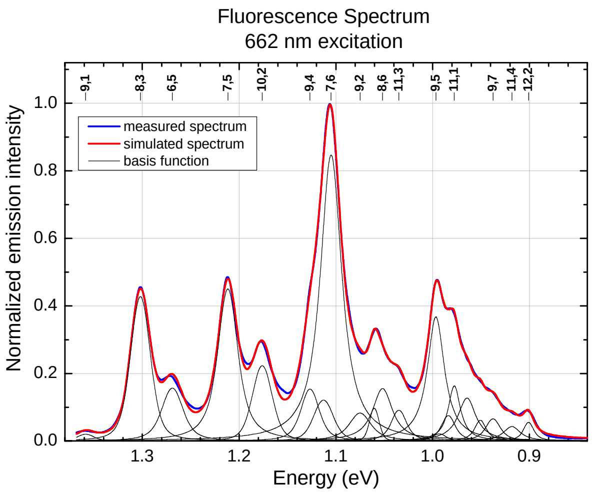


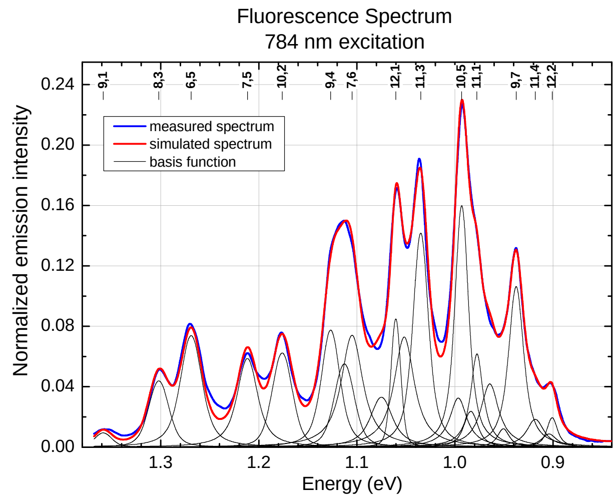


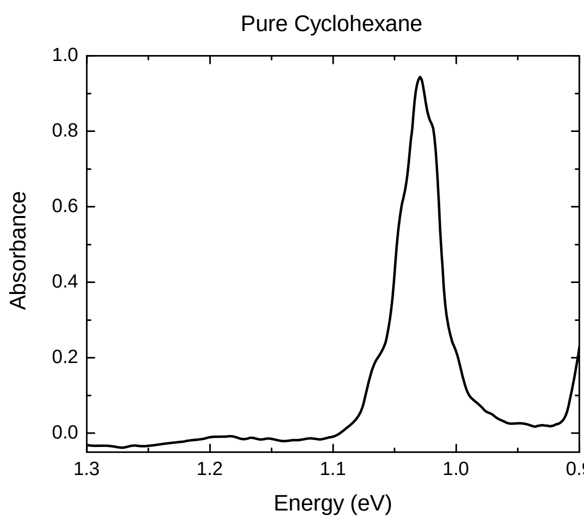
Type	E_{11} (eV)	E_{11} Shift (meV)[a]
(8, 3)	1.302	66
(6, 5)	1.269	83
(7, 5)	1.211	63
(10, 2)	1.176	48
(9, 4)	1.127	44
(7, 6)	1.105	55
(12, 1)	1.060	33
(8, 6)	1.051	49
(11, 3)	1.035	33
(9, 5)	0.997	46
(10, 5)	0.993	31
(11, 1)	0.978	80
(9, 7)	0.938	30
(12, 2)	0.901	50

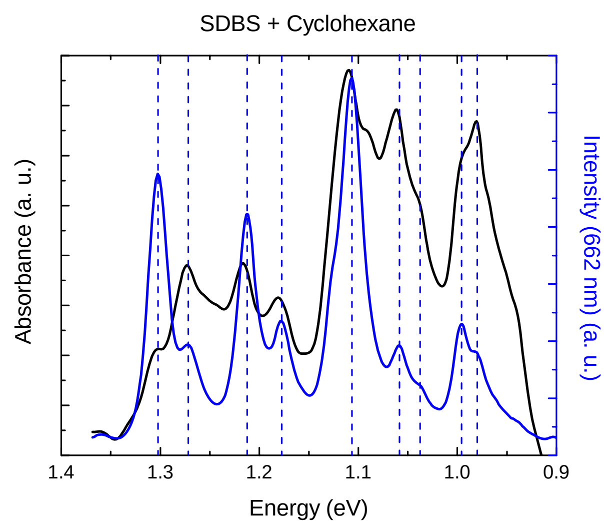
[a] Shift in comparison to fluorescence emission for SWNTs in air

Cyclohexane (ε = 2.02, η = 1.43, D = 0, $f(\eta^2)$ = 0.411)





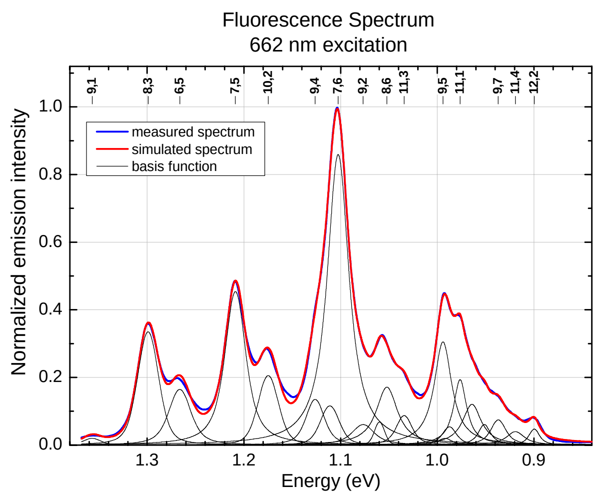


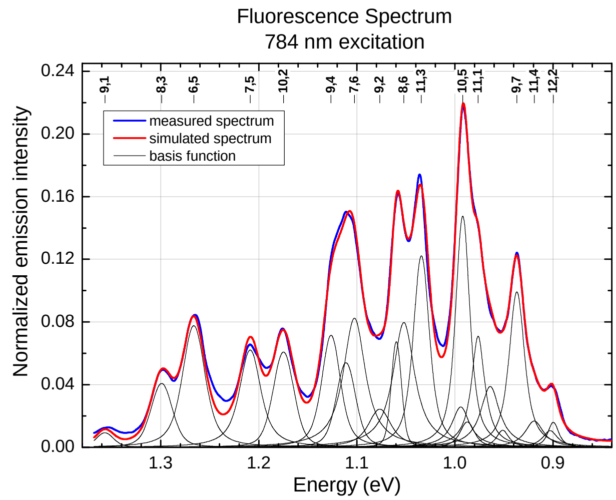


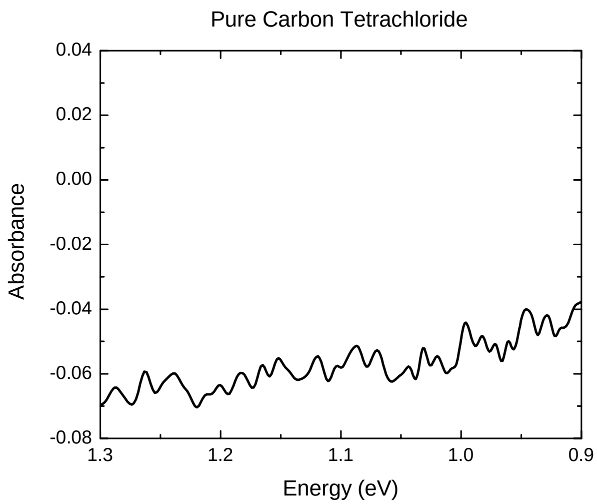
Type	E_{11} (eV)	E_{11} Shift (meV)[a]
(8, 3)	1.302	66
(6, 5)	1.269	83
(7, 5)	1.212	62
(10, 2)	1.176	48
(9, 4)	1.127	44
(7, 6)	1.105	55
(12, 1)	1.060	33
(8, 6)	1.052	48
(11, 3)	1.035	33
(9, 5)	0.997	46
(10, 5)	0.993	31
(11, 1)	0.978	80
(9, 7)	0.938	30
(12, 2)	0.901	50

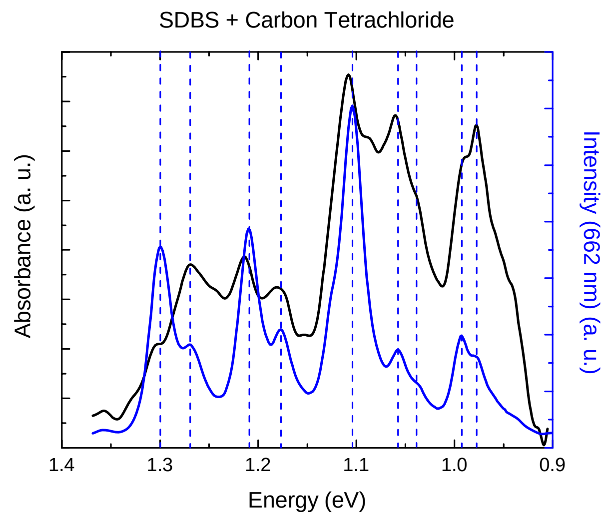
[a] Shift in comparison to fluorescence emission for SWNTs in air

Carbon Tetrachloride ($\varepsilon = 2.23$, $\eta = 1.4$, $D = 0$, $f(\eta^2) = 0.430$)





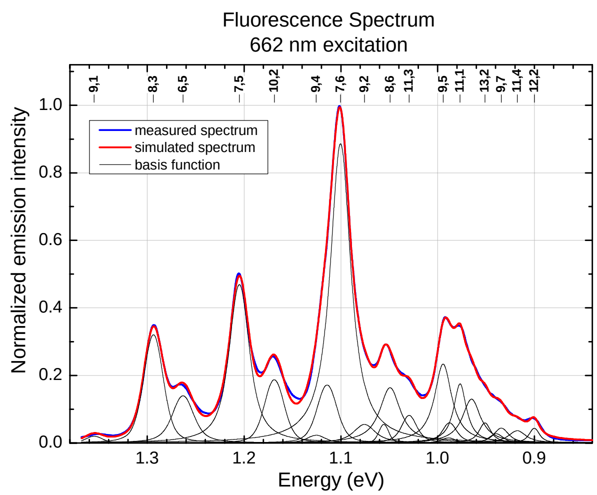


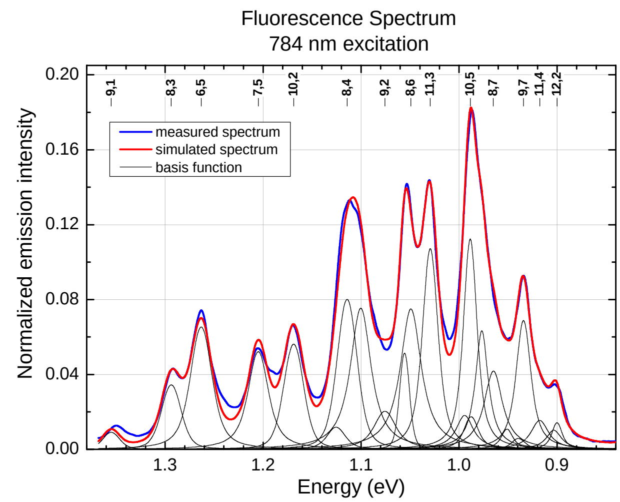


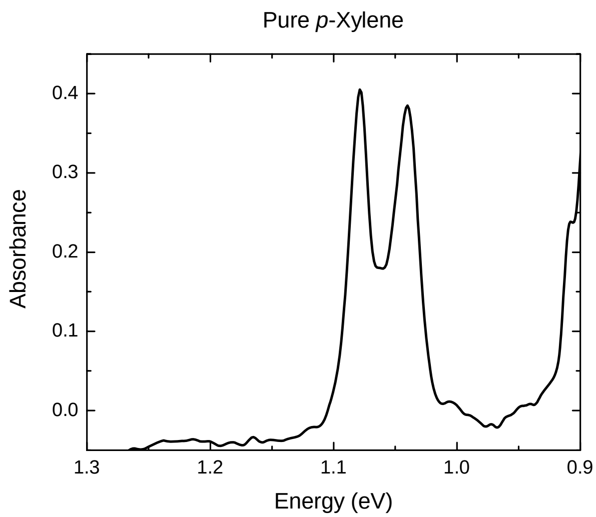
Type	E_{11} (eV)	E_{11} Shift (meV)[a]
(8, 3)	1.299	69
(6, 5)	1.266	86
(7, 5)	1.209	65
(10, 2)	1.175	49
(9, 4)	1.126	45
(7, 6)	1.103	57
(12, 1)	1.060	33
(8, 6)	1.052	48
(11, 3)	1.034	34
(9, 5)	0.994	49
(10, 5)	0.992	32
(11, 1)	0.976	82
(9, 7)	0.937	31
(12, 2)	0.900	51

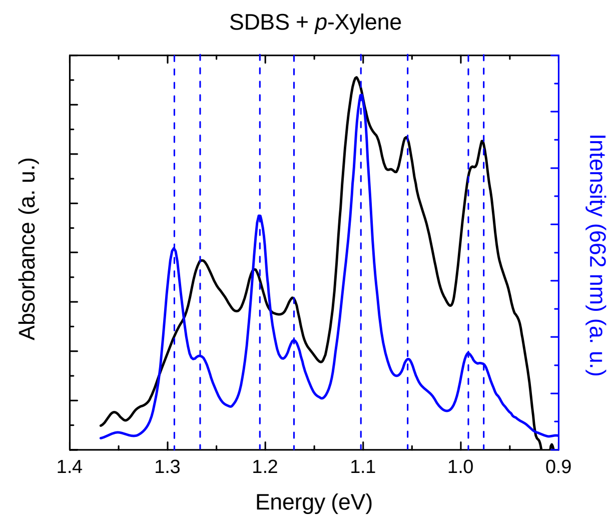
[a] Shift in comparison to fluorescence emission for SWNTs in air

p-Xylene (ε = 2.27, η = 1.50, D = 0, $f(\eta^2)$ = 0.455)





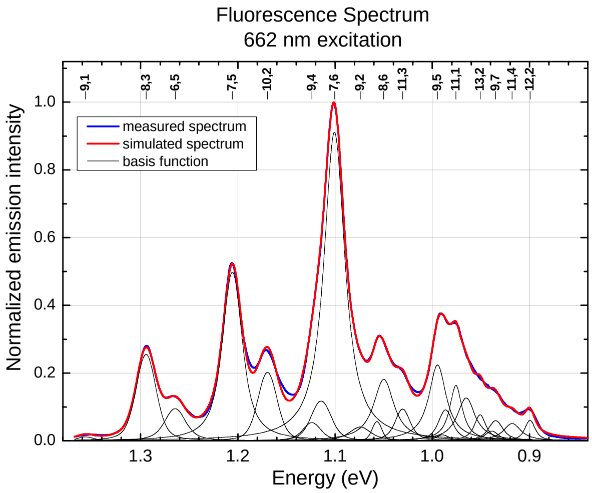


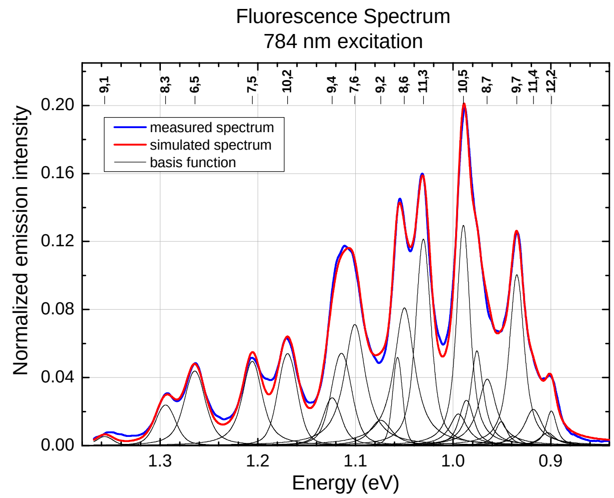


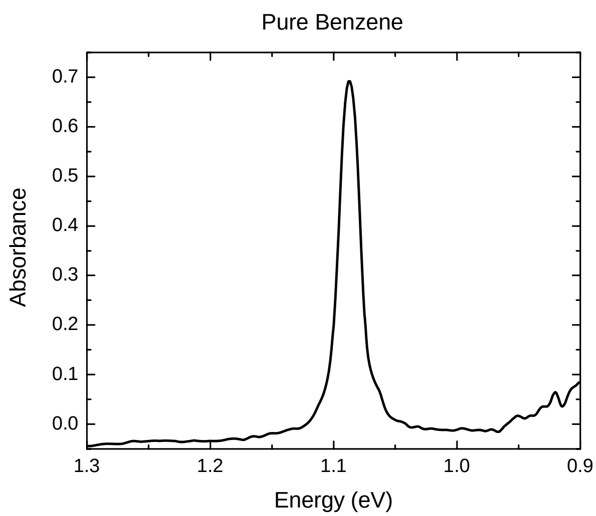
Type	E_{11} (eV)	E_{11} Shift (meV)[a]
(8, 3)	1.294	74
(6, 5)	1.263	89
(7, 5)	1.205	69
(10, 2)	1.169	55
(9, 4)	1.125	46
(7, 6)	1.100	60
(12, 1)	1.056	37
(8, 6)	1.049	51
(11, 3)	1.029	39
(9, 5)	0.994	49
(10, 5)	0.989	35
(11, 1)	0.977	81
(9, 7)	0.934	34
(12, 2)	0.900	51

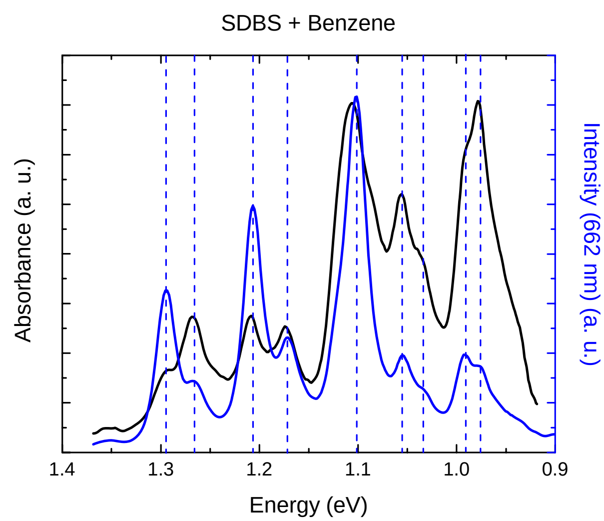
[a] Shift in comparison to fluorescence emission for SWNTs in air

Benzene (ε = 2.28, η = 1.50, D = 0, $f(\eta^2)$ = 0.455)





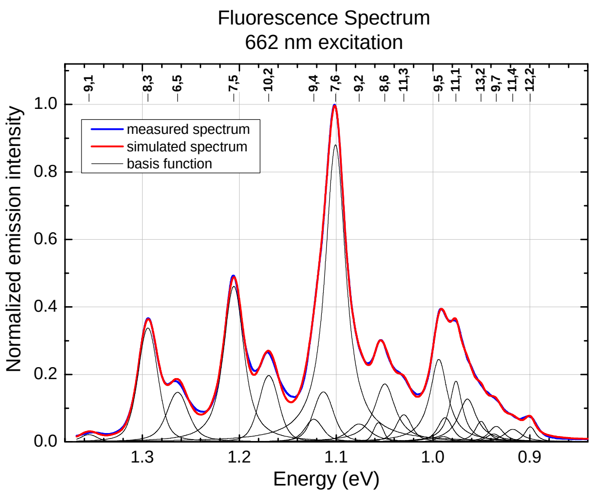


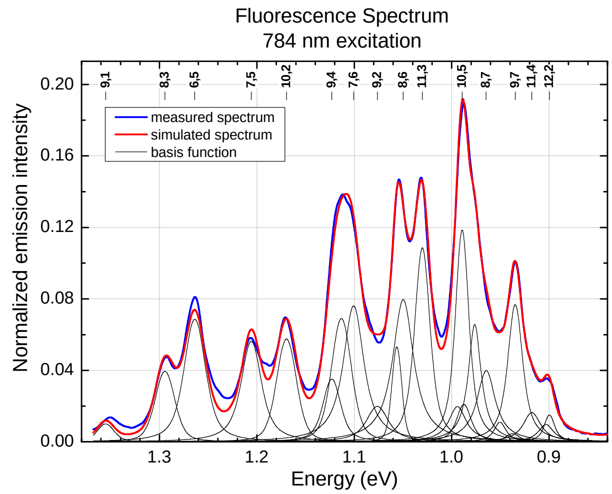


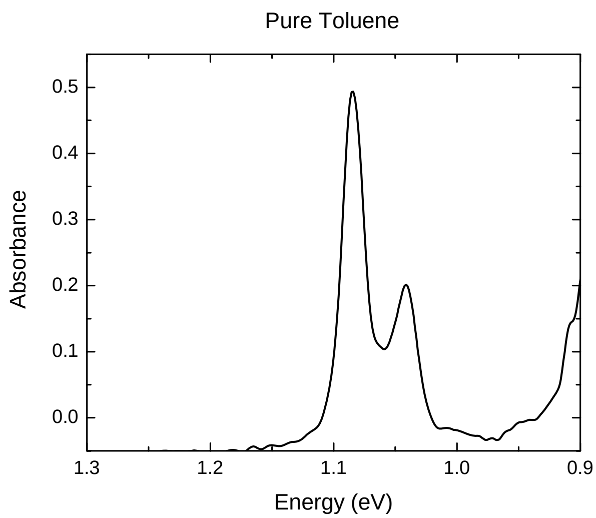
Type	E_{11} (eV)	E_{11} Shift (meV)[a]
(8, 3)	1.294	74
(6, 5)	1.265	87
(7, 5)	1.206	68
(10, 2)	1.170	54
(9, 4)	1.124	47
(7, 6)	1.101	59
(12, 1)	1.057	36
(8, 6)	1.050	50
(11, 3)	1.031	37
(9, 5)	0.995	48
(10, 5)	0.990	34
(11, 1)	0.976	82
(9, 7)	0.935	33
(12, 2)	0.899	52

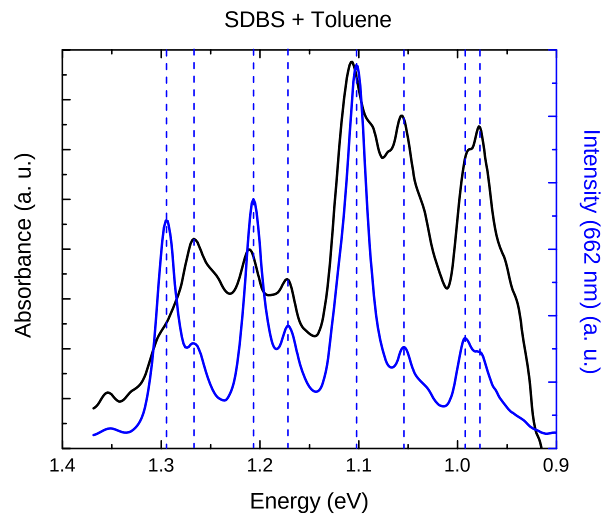
[a] Shift in comparison to fluorescence emission for SWNTs in air

Toluene (ε = 2.39, η = 1.50, D = 0.38, $f(\eta^2)$ = 0.455)





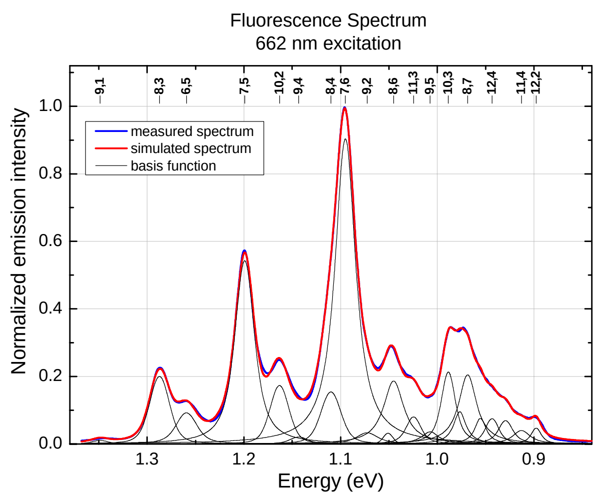


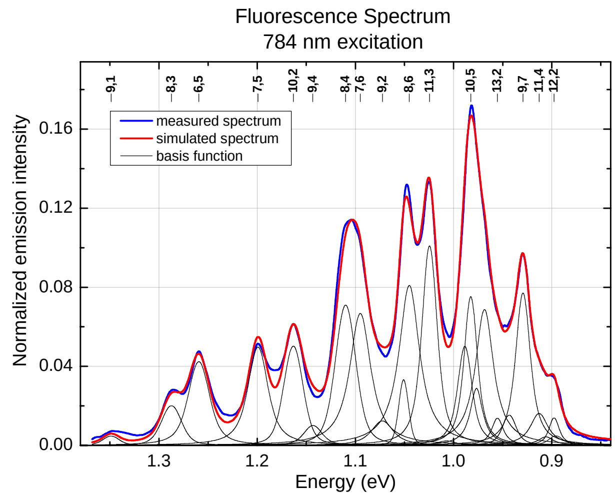


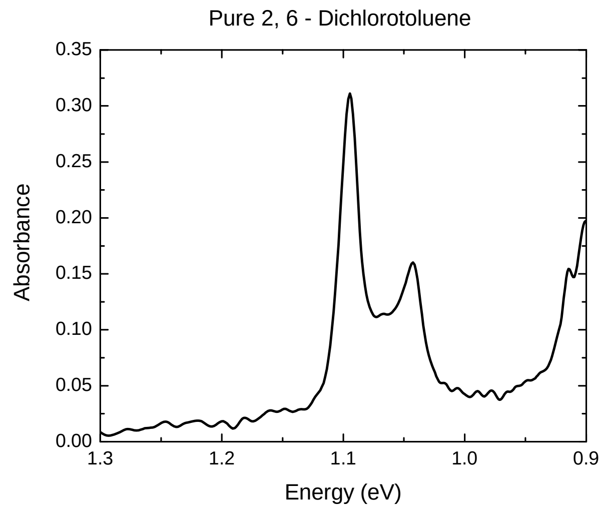
Type	**E_{11} (eV)**	**E_{11} Shift (meV)[a]**
(8, 3)	1.294	74
(6, 5)	1.264	88
(7, 5)	1.206	68
(10, 2)	1.170	54
(9, 4)	1.123	48
(7, 6)	1.101	59
(12, 1)	1.056	37
(8, 6)	1.050	50
(11, 3)	1.030	38
(9, 5)	0.994	49
(10, 5)	0.989	35
(11, 1)	0.976	82
(9, 7)	0.935	33
(12, 2)	0.900	51

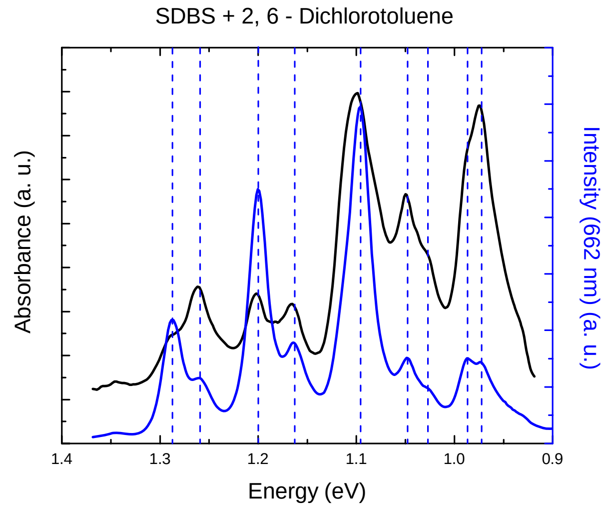
[a] Shift in comparison to fluorescence emission for SWNTs in air

<u>2, 6-Dichlorotoluene</u> (ε = 3.36, η = 1.55, D = 0.83, $f(\eta^2)$ = 0.483)





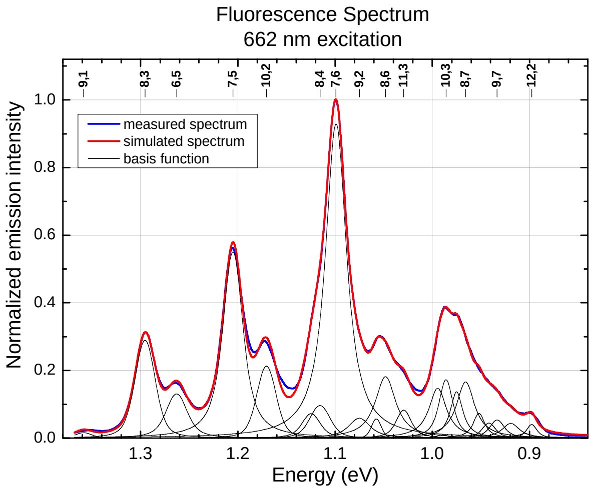


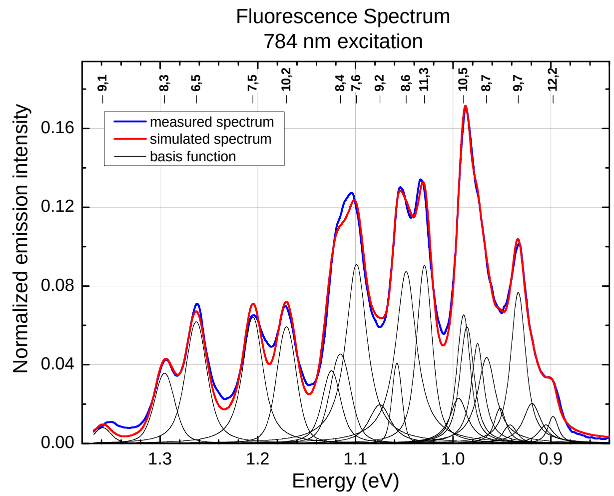


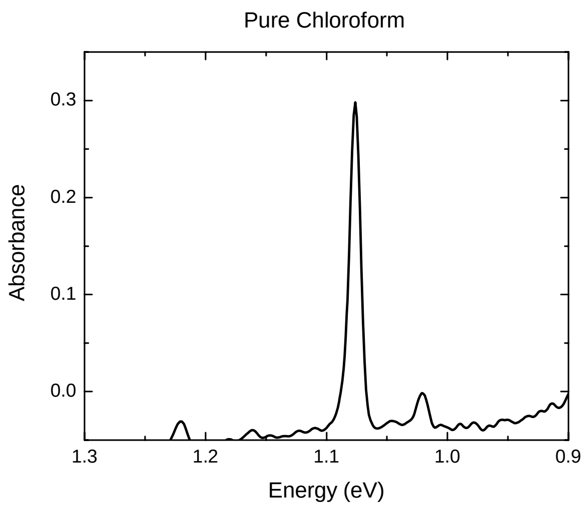
Type	E_{11} (eV)	E_{11} Shift (meV)[a]
(8, 3)	1.287	81
(6, 5)	1.259	93
(7, 5)	1.199	75
(10, 2)	1.163	61
(9, 4)	1.143	28
(7, 6)	1.095	65
(12, 1)	1.051	42
(8, 6)	1.045	55
(11, 3)	1.024	44
(9, 5)	1.007	36
(10, 5)	0.983	41
(11, 1)	0.977	81
(9, 7)	0.929	39
(12, 2)	0.898	53

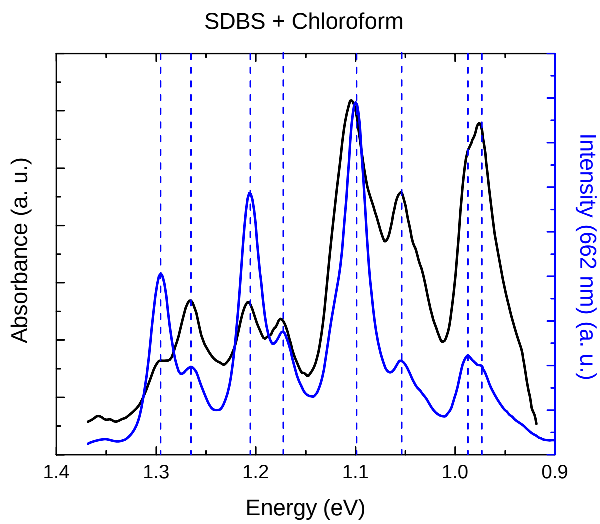
[a] Shift in comparison to fluorescence emission for SWNTs in air

Chloroform (ε = 4.81, η = 1.45, D = 1.04, $f(\eta^2)$ = 0.424)





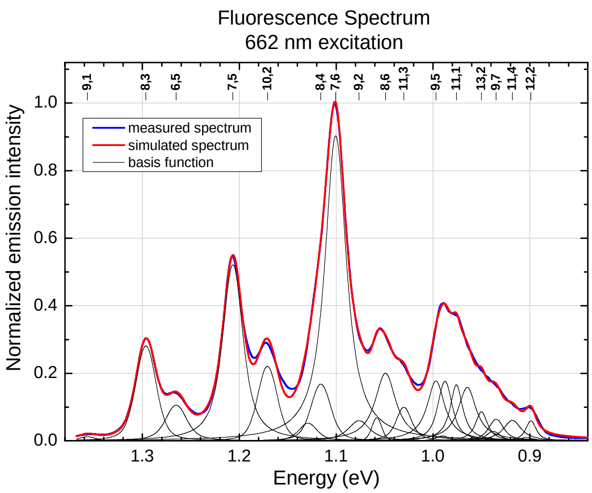


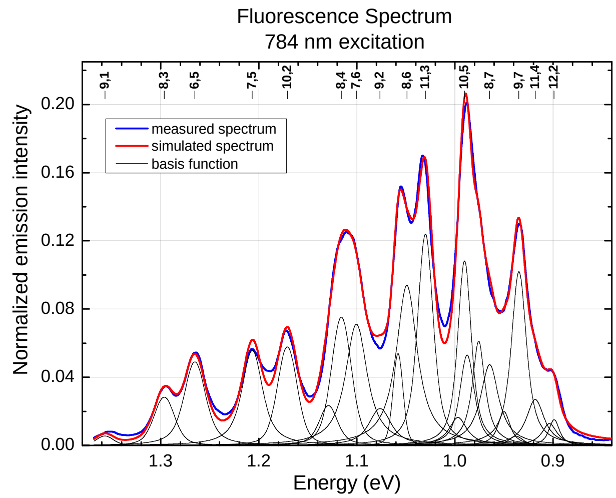


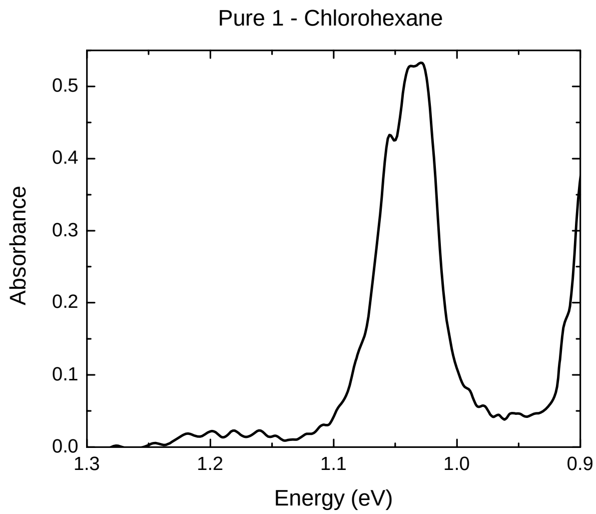
Type	E_{11} (eV)	E_{11} Shift (meV)[a]
(8, 3)	1.295	73
(6, 5)	1.263	89
(7, 5)	1.205	69
(10, 2)	1.171	53
(9, 4)	1.125	46
(7, 6)	1.099	61
(12, 1)	1.058	35
(8, 6)	1.048	52
(11, 3)	1.029	39
(9, 5)	0.994	49
(10, 5)	0.989	35
(11, 1)	0.975	83
(9, 7)	0.933	35
(12, 2)	0.898	53

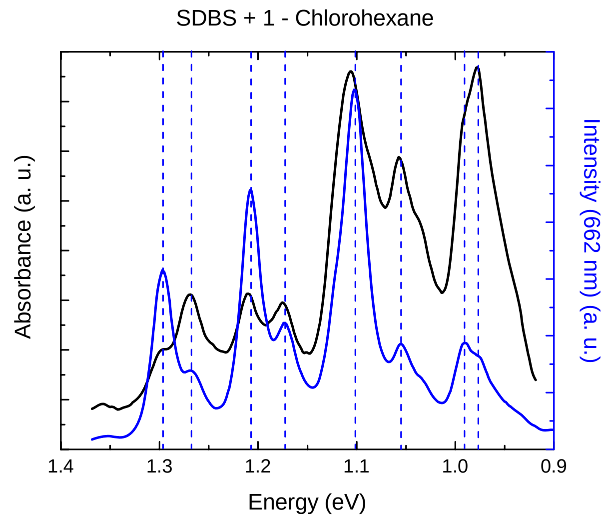
[a] Shift in comparison to fluorescence emission for SWNTs in air

1-Chlorohexane (ε = 6.10, η = 1.42, D = 1.94, $f(\eta^2)$ = 0.404)





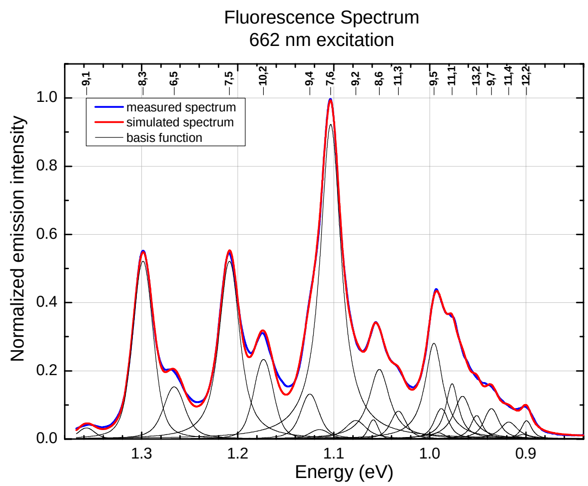


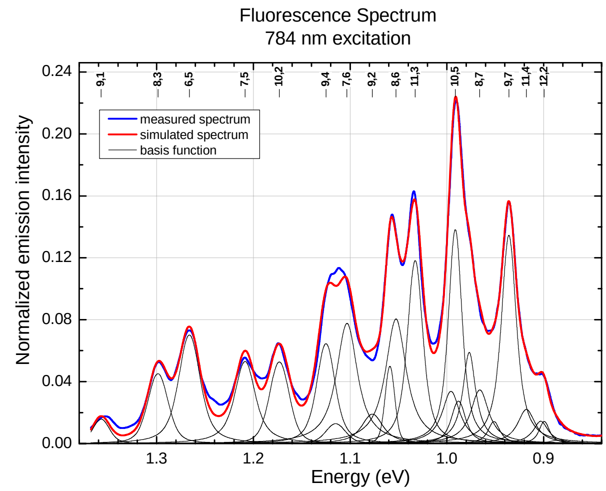


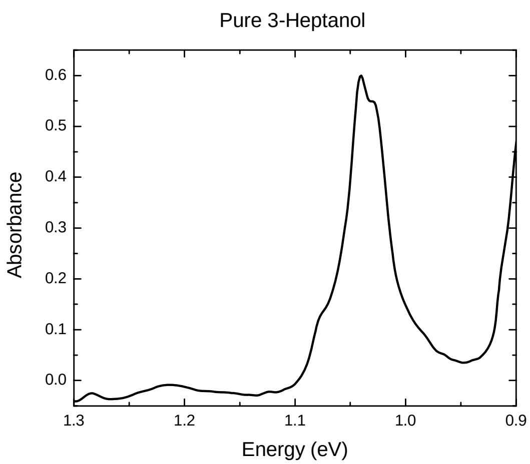
Type	E_{11} (eV)	E_{11} Shift (meV)[a]
(8, 3)	1.296	72
(6, 5)	1.265	87
(7, 5)	1.207	67
(10, 2)	1.171	53
(9, 4)	1.129	42
(7, 6)	1.100	60
(12, 1)	1.058	35
(8, 6)	1.049	51
(11, 3)	1.030	38
(9, 5)	0.997	46
(10, 5)	0.990	34
(11, 1)	0.976	82
(9, 7)	0.935	33
(12, 2)	0.899	52

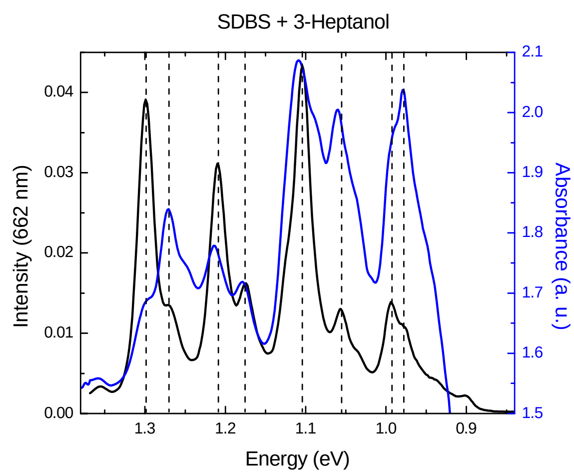
[a] Shift in comparison to fluorescence emission for SWNTs in air

3-Heptanol (ε = 7.07, η = 1.42, D = 1.71, $f(\eta^2)$ = 0.404)





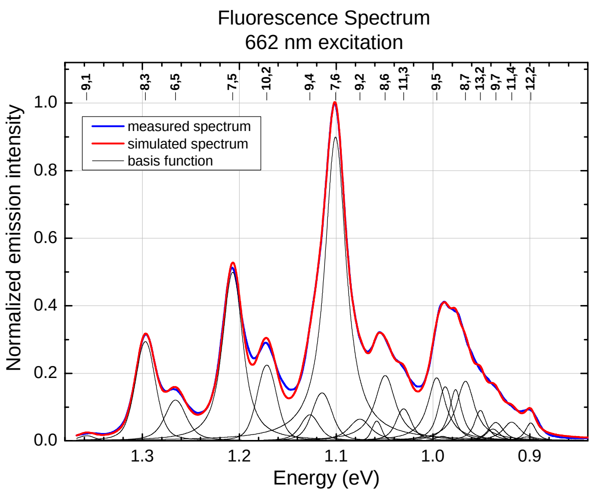


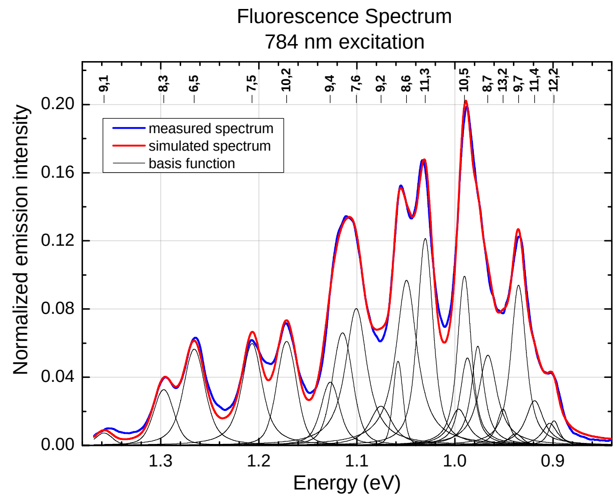


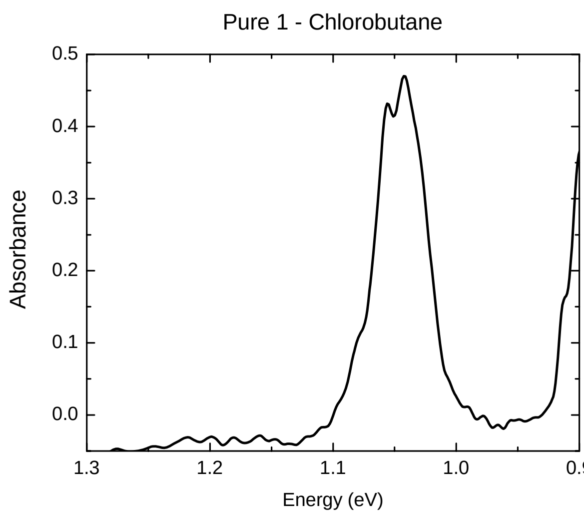
Type	E_{11} (eV)	E_{11} Shift (meV)[a]
(8, 3)	1.299	69
(6, 5)	1.267	85
(7, 5)	1.209	65
(10, 2)	1.173	51
(9, 4)	1.126	45
(7, 6)	1.102	58
(12, 1)	1.059	34
(8, 6)	1.05	50
(11, 3)	1.033	35
(9, 5)	0.995	48
(10, 5)	0.992	32
(11, 1)	0.976	82
(9, 7)	0.936	32
(12, 2)	0.900	51

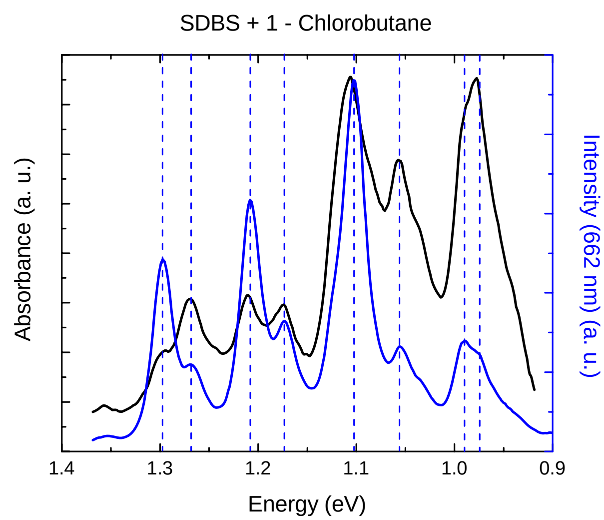
[a] Shift in comparison to fluorescence emission for SWNTs in air

1-Chlorobutane (ε = 7.28, η = 1.40, D = 2.05, $f(\eta^2)$ = 0.390)





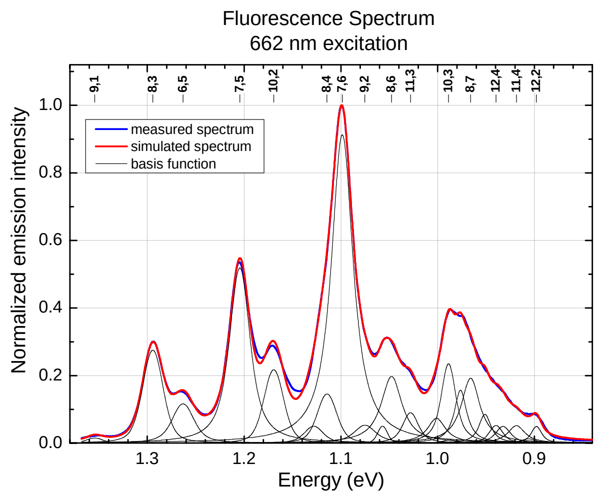


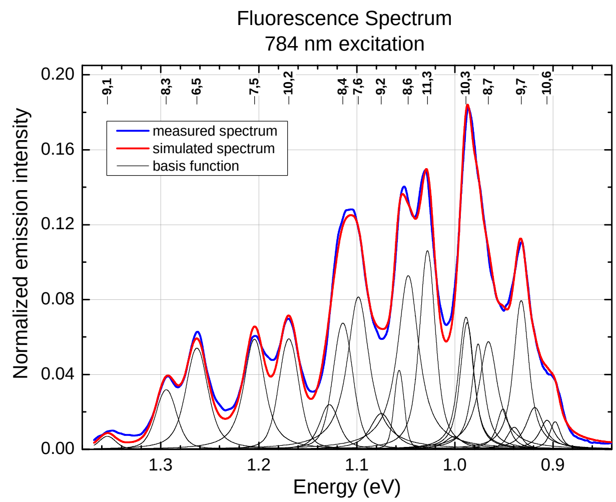


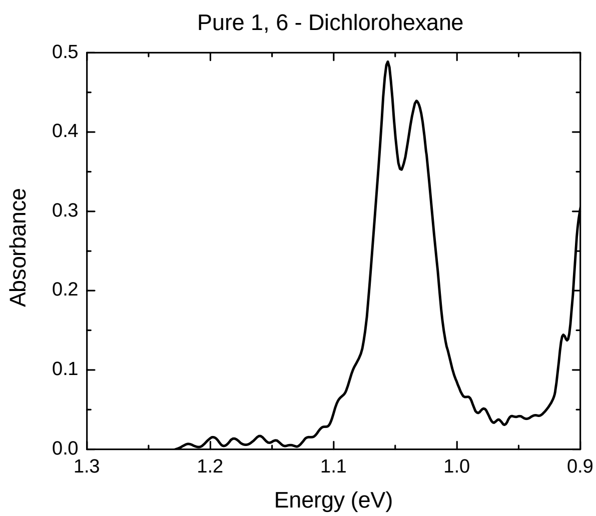
Type	E_{11} (eV)	E_{11} Shift (meV)[a]
(8, 3)	1.297	71
(6, 5)	1.266	86
(7, 5)	1.207	67
(10, 2)	1.172	52
(9, 4)	1.127	44
(7, 6)	1.101	59
(12, 1)	1.058	35
(8, 6)	1.049	51
(11, 3)	1.030	38
(9, 5)	0.996	47
(10, 5)	0.990	34
(11, 1)	0.977	81
(9, 7)	0.935	33
(12, 2)	0.899	52

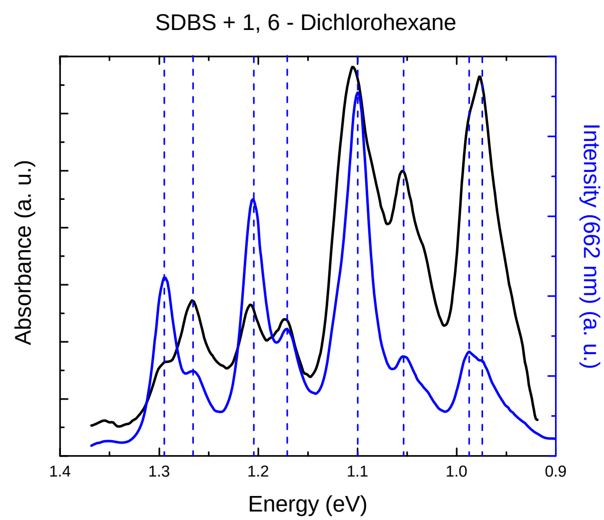
[a] Shift in comparison to fluorescence emission for SWNTs in air

1, 6-Dichlorohexane (ε = 8.60, η = 1.46, D = 2.03, $f(\eta^2)$ = 0.430)





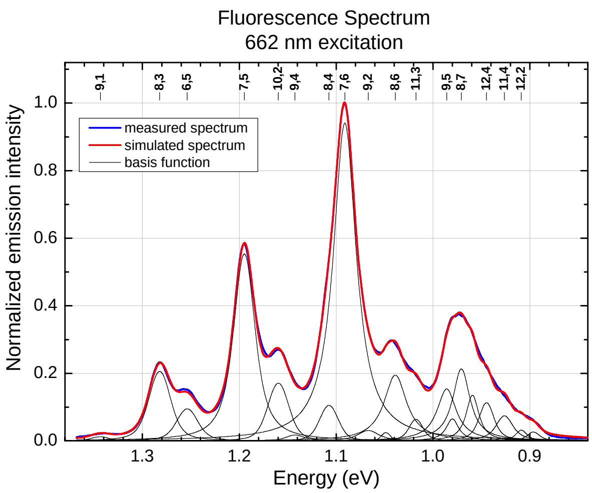


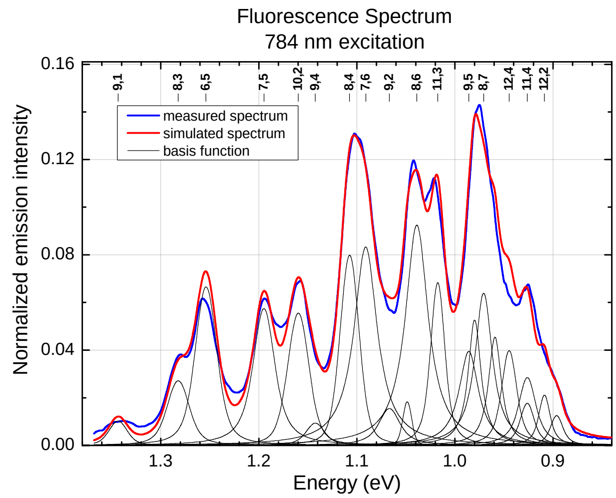


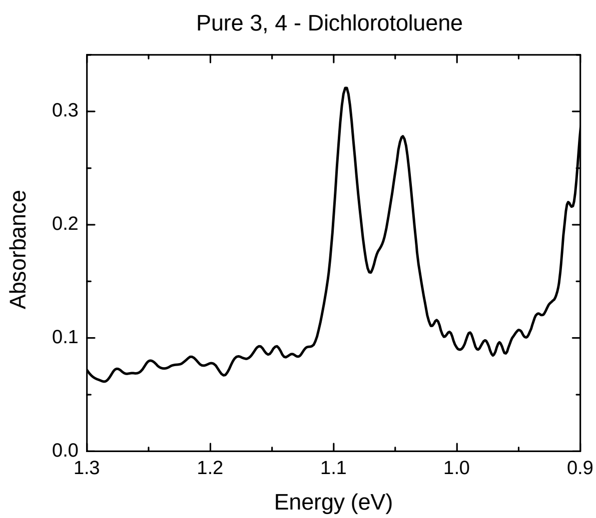
Type	E_{11} (eV)	E_{11} Shift (meV)[a]
(8, 3)	1.294	74
(6, 5)	1.263	89
(7, 5)	1.204	70
(10, 2)	1.169	55
(9, 4)	1.128	43
(7, 6)	1.099	61
(12, 1)	1.057	36
(8, 6)	1.048	52
(11, 3)	1.028	40
(9, 5)	1.001	42
(10, 5)	0.988	36
(11, 1)	0.976	82
(9, 7)	0.932	36
(12, 2)	0.898	53

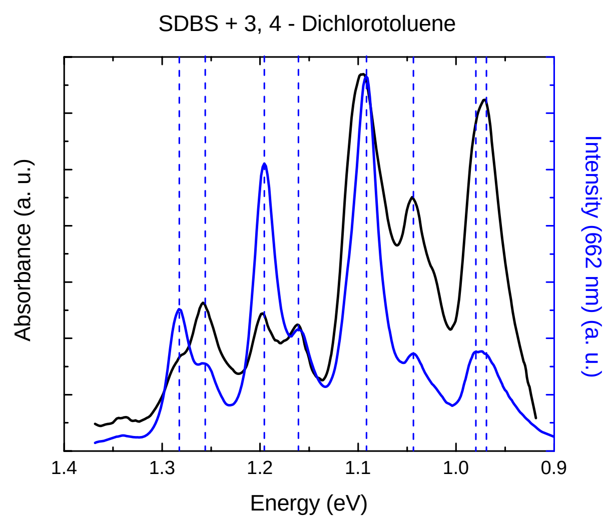
[a] Shift in comparison to fluorescence emission for SWNTs in air

<u>3, 4-Dichlorotoluene</u> (ε = 9.39, η = 1.55, D = 3.00, $f(\eta^2)$ = 0.483)





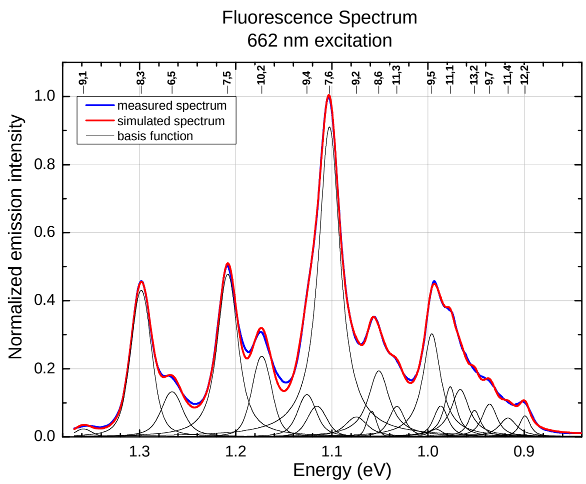


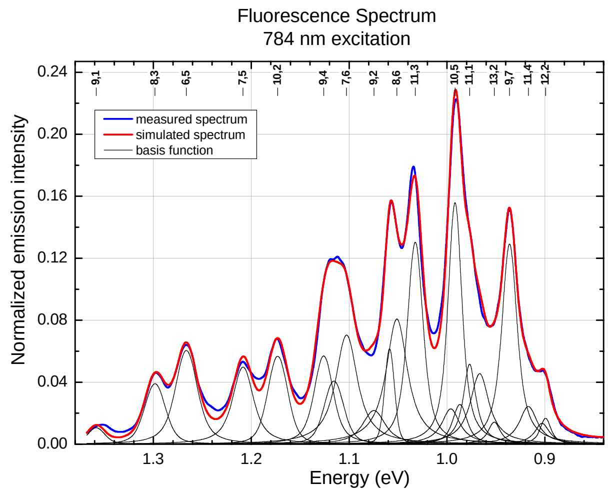


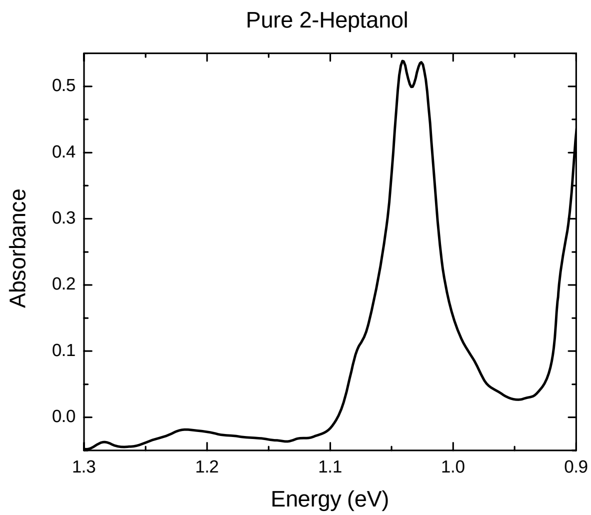
Type	**E_{11} (eV)**	**E_{11} Shift (meV)[a]**
(8, 3)	1.282	86
(6, 5)	1.254	98
(7, 5)	1.195	79
(10, 2)	1.160	64
(9, 4)	1.142	29
(7, 6)	1.091	69
(12, 1)	1.049	44
(8, 6)	1.039	61
(11, 3)	1.018	50
(9, 5)	0.986	57
(11, 1)	0.980	78
(9, 7)	0.926	42
(12, 2)	0.909	42

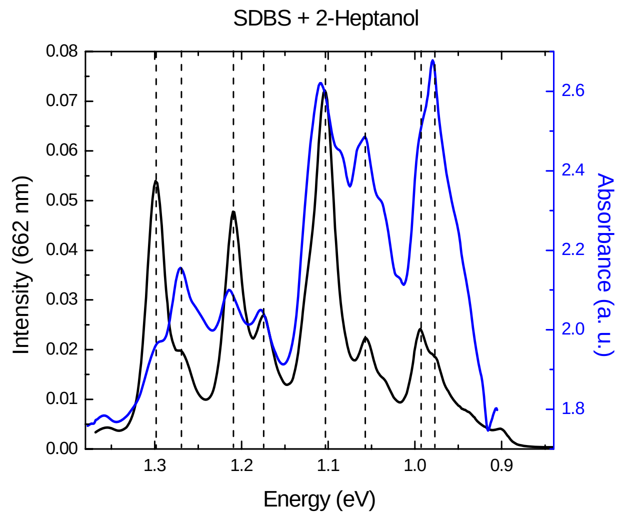
[a] Shift in comparison to fluorescence emission for SWNTs in air

2-Heptanol ($\varepsilon = 9.72$, $\eta = 1.42$, $D = 1.71$, $f(\eta^2) = 0.404$)





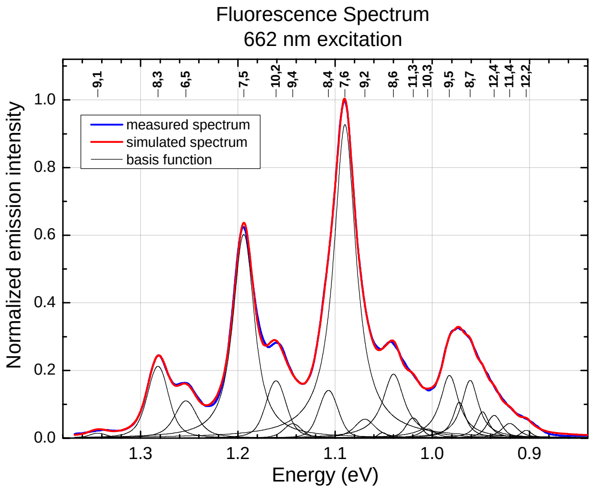


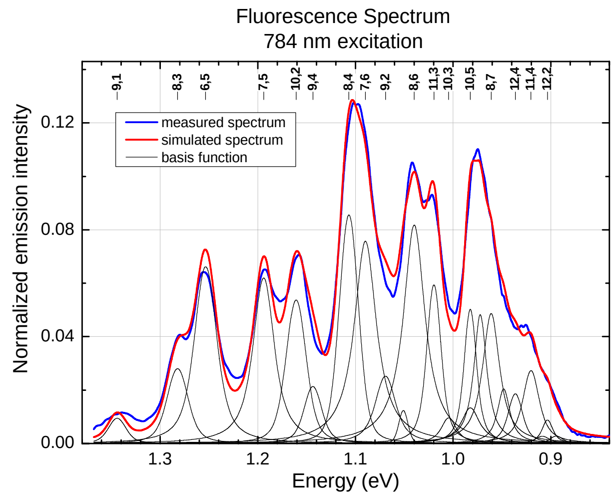


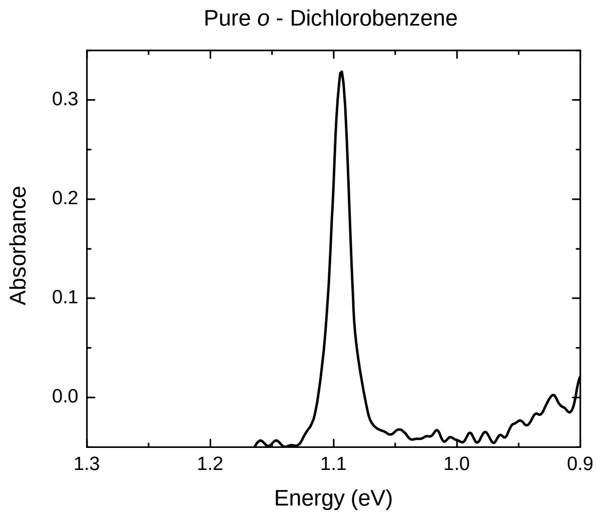
Type	E_{11} (eV)	E_{11} Shift (meV)[a]
(8, 3)	1.299	69
(6, 5)	1.267	85
(7, 5)	1.209	65
(10, 2)	1.173	51
(9, 4)	1.126	45
(7, 6)	1.102	58
(12, 1)	1.059	34
(8, 6)	1.05	50
(11, 3)	1.033	35
(9, 5)	0.995	48
(10, 5)	0.992	32
(11, 1)	0.976	82
(9, 7)	0.936	32
(12, 2)	0.900	51

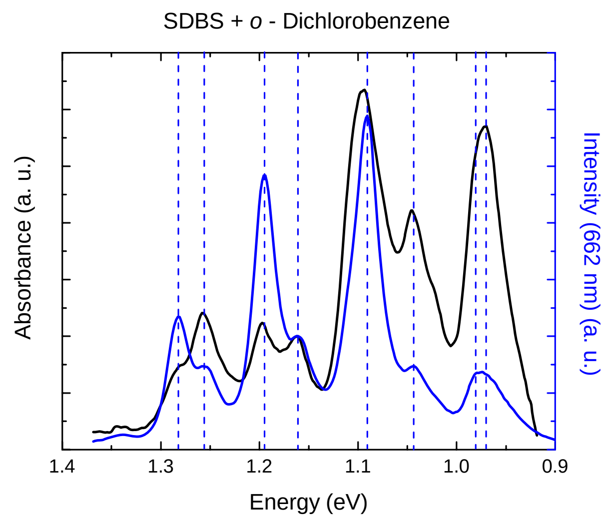
[a] Shift in comparison to fluorescence emission for SWNTs in air

_o_-Dichlorobenzene (ε = 10.12, η = 1.55, D = 2.50, $f(\eta^2)$ = 0.483)









Type	E_{11} (eV)	E_{11} Shift (meV)[a]
(8, 3)	1.282	86
(6, 5)	1.253	99
(7, 5)	1.194	80
(10, 2)	1.161	63
(9, 4)	1.144	27
(7, 6)	1.090	70
(12, 1)	1.051	42
(8, 6)	1.040	60
(11, 3)	1.020	48
(9, 5)	0.982	61
(10, 5)	0.982	42
(11, 1)	0.972	86
(12, 2)	0.903	48

[a] Shift in comparison to fluorescence emission for SWNTs in air