

Contents

1	Introduction	1
	References	6
2	Methods	9
2.1	Excitonic Models	9
2.2	Energy Transfer and Dissipation	12
2.2.1	Description of the Bath	14
2.2.2	Bloch-Redfield Theory	15
2.3	2D Electronic Spectroscopy	20
2.3.1	Experimental Setup	21
2.3.2	Theory Behind 2D Electronic Spectroscopy	22
2.3.3	Interpreting 2D Spectra	26
	References	31
3	2D Spectroscopy of Pentacene Thin Films	33
3.1	Structure of Pentacene	34
3.2	Singlet Fission	36
3.3	Experimental Results	37
3.3.1	2D Spectra	39
3.3.2	Waiting Time Dynamics	39
3.4	Vibronic Model	43
3.4.1	Model	43
3.4.2	Eigenstates	45
3.5	Ultrafast Dynamics	47
3.6	Simulation of Beating Maps	49
3.7	Discussion of Beating Maps	50
3.8	Analysing the Oscillation Signs	53
3.9	Summary and Conclusions	55
	References	57

4	Time-Frequency Analysis for 2D Spectroscopy of PSII	59
4.1	Photosystem II	60
4.1.1	Structure	61
4.1.2	Function	63
4.2	Wavelet Analysis	64
4.2.1	Wavelet Analysis Method	64
4.2.2	Distinguishing Amplitude Modulation from Interference Using Artificial Signals	65
4.2.3	Waiting Time at Which the Oscillation Frequency Amplitude Modulation Occurs	68
4.2.4	Changing Position in the 2D Spectrum	69
4.3	Wavelet Analysis for PSII 2DES Data	72
4.3.1	Experimental Results	72
4.3.2	Discussion	73
4.4	Conclusion	78
	References.	79
5	Nonlinear Network Model of Energy Transfer and Localisation in FMO	81
5.1	Structure of FMO	82
5.2	Network Models	84
5.3	Normal Modes	86
5.4	Dynamics	89
5.5	Optical Spectra	94
5.6	Conclusion	98
	References.	99
6	Conclusions	103
	References.	105
	Appendix A: The Density Matrix and Reduced Density Matrix	107
	Appendix B: Interaction Picture	109

Ultrafast Quantum Effects and Vibrational Dynamics in
Organic and Biological Systems

Morgan, S.E.

2017, XV, 110 p. 72 illus., 65 illus. in color., Hardcover

ISBN: 978-3-319-63398-5