

# *Resonance Energy Transfer*

**David L. Andrews**

*University of East Anglia, UK*

and

**Andrey A. Demidov**

*Northeastern University, Boston, USA*

**JOHN WILEY & SONS**

Chichester • New York • Weinheim • Brisbane • Singapore • Toronto

# Contents

<b>List of Contributors</b>	ix
<b>Preface</b>	xv
<b>Foreword</b>	
<i>Graham R. Fleming</i>	xvii
<b>1 Resonance energy transfer in proteins</b>	
<i>Cristobal G. dos Remedios and Pierre D. J. Moens</i>	1
1.1 Introduction	1
1.2 Some basic considerations	2
1.3 A short history of FRET determinations	4
1.4 The components of the Förster equation	6
1.5 Quantum yield	8
1.6 Determining the spectral overlap	11
1.7 Steady state or time-resolved measurements?	11
1.8 Resonance energy transfer using intrinsic amino acids	12
1.9 Homotransfer between intrinsic probes	14
1.10 Heterotransfer	16
1.11 The range of distances determined by resonance energy transfer	23
1.12 Precise location of resonance energy transfer probes	25
1.13 Properties of probes	25
1.14 Labeling specific residues in proteins	30
1.15 Resonance energy transfer experiments using lanthanide ions	37
1.16 Measurements in radially symmetrical systems	41
1.17 Comparison with crystallographic distances	46
1.18 Using resonance energy transfer to constrain molecular models	47
1.19 Resonance energy transfer with single fluorophores: new wave experiments	47

1.20	Intramolecular energy transfer in proteins bound to membranes	48
1.21	Green fluorescent protein	49
1.22	Resonance energy transfer and biosensors: a new and promising technology	51
1.23	Shortcomings	52
1.24	The future of FRET	54
1.25	Summary	54
	Dedication	55
	Acknowledgments	55
	References	55
<b>2</b>	<b>Unified theory of radiative and radiationless energy transfer</b>	
	<i>Gediminas Juzeliūnas and David L. Andrews</i>	<b>65</b>
2.1	Introduction	65
2.2	Background	66
2.3	The basis of the unified theory	69
2.4	Spectral features	76
2.5	Refraction and dissipation	82
2.6	Dynamics of energy transfer between a pair of molecules in a dielectric medium	92
2.7	Conclusion	102
	Appendix A: Heitler–Ma method for analysis of the transition operator	103
	Appendix B: Modified approach to the transition operator	104
	Acknowledgment	104
	References	104
<b>3</b>	<b>Dynamics of radiative transport</b>	
	<i>Mário N. Berberan-Santos, Eduardo J. Nunes Pereira, and José M. G. Martinho</i>	<b>108</b>
3.1	Introduction	108
3.2	Overview of atomic and molecular radiative transport	109
3.3	The Holstein–Biberman equation	112
3.4	Multiple scattering representation	121
3.5	Stochastic approach	124
3.6	Combined radiative and nonradiative transport	137
3.7	Conclusion	142
	Appendix A: Probability of emission of a photon between $t$ and $t + dt$ for an $n$ th-generation molecule	143
	Appendix B: Depolarization factor for radiative transfer according to classical electrodynamics	143
	References	146

<b>4</b>	<b>Orientational aspects in pair energy transfer</b>	
	<i>B. Wieb van der Meer</i>	<b>151</b>
4.1	Introduction	151
4.2	$\kappa^2$ and probability	156
4.3	$\kappa^2$ and anisotropy	165
4.4	Notes on the effects of order and motion	170
	Acknowledgments	171
	References	171
<b>5</b>	<b>Polarization in molecular complexes with incoherent energy transfer</b>	
	<i>Andrey A. Demidov and David L. Andrews</i>	<b>173</b>
5.1	Introduction	173
5.2	Interaction of light with single molecules or chromophores	174
5.3	Bichromophore molecular complexes	180
5.4	Trichromophore complexes	190
5.5	Multichromophore complexes with $C_3$ symmetry	193
5.6	Conclusion	202
	Appendix A	203
	Appendix B	206
	Appendix C	207
	Appendix D	207
	References	209
<b>6</b>	<b>Theory of coupling in multichromophoric systems</b>	
	<i>Gregory D. Scholes</i>	<b>212</b>
6.1	Introduction	212
6.2	Reactant and product states: LMO model	216
6.3	The origin of coupling matrix elements	220
6.4	Paradigmatic results	223
6.5	Coulombic coupling	228
6.6	Superexchange	234
6.7	Interpretation of steady state spectra	236
6.8	Calculation of couplings	238
	Acknowledgements	240
	References	240
<b>7</b>	<b>Exciton annihilation in molecular aggregates</b>	
	<i>Leonas Valkunas, Gediminas Trinkunas, and Vladas Liuolia</i>	<b>244</b>
7.1	Introduction	244
7.2	Theory	247
7.3	Applications	279
7.4	Discussion	298
	Acknowledgments	301
	References	301

<b>8</b>	<b>Energy transfer and localization: applications to photosynthetic systems</b>	
	<i>Sandrasegaram Gnanakaran, Gilad Haran, Ranjit Kumble, and Robin M. Hochstrasser</i>	<b>308</b>
8.1	Introduction	308
8.2	Optical properties of dimers and aggregates	309
8.3	Energy transfer and localization in antenna complexes and reaction centers	335
	Acknowledgments	355
	References	355
<b>9</b>	<b>Excitation energy transfer in photosynthesis</b>	
	<i>Rienk van Grondelle and Oscar J. G. Somsen</i>	<b>366</b>
9.1	Introduction	366
9.2	The structure of light-harvesting complexes	368
9.3	The mechanism of energy transfer and trapping in photosynthesis	374
9.4	Dynamics of excitation energy transfer	382
9.5	Conclusions	390
	Acknowledgments	390
	References	391
<b>10</b>	<b>The Fenna–Matthews–Olson protein: a strongly coupled photosynthetic antenna</b>	
	<i>Sergei Savikhin, Daniel R. Buck, and Walter S. Struve</i>	<b>399</b>
10.1	Introduction	399
10.2	Steady state spectroscopy	402
10.3	FMO exciton simulations	403
10.4	FMO primary processes	410
10.5	Epilog and future prospects	429
	Acknowledgments	430
	References	431
<b>11</b>	<b>Use of a Monte Carlo method in the problem of energy migration in molecular complexes</b>	
	<i>Andrey A. Demidov</i>	<b>435</b>
11.1	Introduction	435
11.2	An illustration of Monte Carlo calculations in the problem of fluorescence decay	437
11.3	Energy transfer in CME: major algorithm	439
11.4	Applications of Monte Carlo simulations	446
11.5	Conclusion	463
	Acknowledgments	464
	References	464
	Index	467