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An 'all pigment' model of excitation quenching in LHCII

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Electronic Supplementary Information

Table S1 Inter-pigment hopping times (in ps), obtained assuming Förster regime and two domains of strongly-coupled Chls. Inter-Chl couplings were taken from Müh et al.[1] Values longer than 1 ns are denoted as "Inf".

Pigments	Chl b 601	Chl a 602	Chl a 603	Chl a 604	Chl b 605	Chl b 606	Chl b 607	Chl b 608	Chl b 609	Chl a 610-611-612	Chl a 613-614	Lut 620	Lut 621	Vio 622	Neo 623
Chl b 601	–	26.3	Inf	Inf	335.6	92.4	137.4	152.2	21.3	139.1	Inf	Inf	Inf	Inf	Inf
Chl a 602	2.7	–	2.5	19.5	Inf	119.5	26.7	25.0	10.2	22.1	228.0	Inf	Inf	Inf	Inf
Chl a 603	275.4	1.6	–	385.1	Inf	369.0	49.7	104.2	2.3	17.1	41.2	Inf	Inf	Inf	Inf
Chl a 604	964.5	10.8	332.3	–	865.6	1.5	3.9	129.3	Inf	53.0	85.3	Inf	Inf	Inf	Inf
Chl b 605	450.5	Inf	Inf	Inf	–	6.3	146.3	163.5	Inf	Inf	Inf	Inf	Inf	Inf	Inf
Chl b 606	83.8	Inf	Inf	23.6	4.3	–	4.0	44.7	88.7	Inf	Inf	Inf	Inf	Inf	Inf
Chl b 607	56.8	108.1	313.5	28.2	45.0	1.8	–	22.3	30.7	Inf	522.1	Inf	Inf	Inf	Inf
Chl b 608	59.9	96.4	625.3	899.2	47.9	19.4	21.3	–	1.4	17.4	Inf	Inf	Inf	Inf	Inf
Chl b 609	30.0	141.8	49.2	Inf	Inf	138.1	104.6	5.1	–	Inf	Inf	Inf	Inf	Inf	Inf
Chl a 610-611-612	5.3	5.6	6.8	21.5	Inf	745.7	116.2	1.4	296.7	–	14.4	Inf	Inf	Inf	Inf
Chl a 613-614	83.4	94.2	23.0	55.0	Inf	392.1	56.1	235.4	774.1	22.0	–	Inf	Inf	Inf	Inf
Lut 620	Inf	Inf	Inf	Inf	Inf	Inf	Inf	Inf	Inf	65.8	505.8	–	Inf	Inf	Inf
Lut 621	Inf	343.7	22.5	89.9	Inf	698.2	751.0	Inf	Inf	Inf	Inf	Inf	–	Inf	Inf
Vio 622	Inf	Inf	Inf	Inf	Inf	Inf	Inf	Inf	Inf	Inf	272.5	Inf	Inf	–	Inf
Neo 623	Inf	Inf	Inf	174.7	Inf	186.8	Inf	288.3	Inf	Inf	Inf	Inf	Inf	Inf	–

[1] F. Müh, M.E.A. Madjet and T. Renger, J. Phys. Chem. B, 2010, 114, 13517–13535.

Table S2 Inter-pigment hopping times (in ps), obtained assuming Förster regime and two domains of strongly-coupled Chls. Inter-Chl couplings were taken from our MNDO-CAS-CI calculations. Values longer than 1 ns are denoted as "Inf".

Pigments	Chl b 601	Chl a 602	Chl a 603	Chl a 604	Chl b 605	Chl b 606	Chl b 607	Chl b 608	Chl b 609	Chl a 610-611-612	Chl a 613-614	Lut 620	Lut 621	Vio 622	Neo 623
Chl b 601	–	26.8	Inf	Inf	Inf	147.0	476.7	460.9	57.9	Inf	Inf	Inf	Inf	Inf	Inf
Chl a 602	2.7	–	1.7	17.5	Inf	97.8	38.5	39.3	17.8	8.4	26.8	Inf	Inf	Inf	Inf
Chl a 603	236.8	1.1	–	15.7	Inf	65.5	Inf	140.9	3.0	10.7	24.9	Inf	Inf	Inf	Inf
Chl a 604	Inf	9.7	13.5	–	Inf	1.2	7.2	327.6	341.5	35.4	90.4	Inf	Inf	Inf	Inf
Chl b 605	Inf	Inf	Inf	Inf	–	4.0	Inf	224.1	Inf	Inf	Inf	Inf	Inf	Inf	Inf
Chl b 606	133.3	869.4	906.1	19.8	2.7	–	5.8	123.9	2.1	Inf	Inf	Inf	Inf	Inf	Inf
Chl b 607	197.0	156.1	Inf	52.7	587.4	2.6	–	40.0	19.1	923.3	Inf	Inf	Inf	Inf	Inf
Chl b 608	181.3	151.6	846.1	Inf	65.7	53.8	38.1	–	4.2	18.1	Inf	Inf	Inf	Inf	Inf
Chl b 609	81.7	245.8	64.9	Inf	Inf	3.2	65.2	14.9	–	Inf	Inf	Inf	Inf	Inf	Inf
Chl a 610-611-612	48.9	2.2	4.1	15.1	323.9	65.0	71.9	1.4	317.5	–	4.4	Inf	Inf	Inf	Inf
Chl a 613-614	168.3	11.9	13.3	57.5	Inf	964.1	176.4	625.7	Inf	6.9	–	Inf	Inf	Inf	Inf
Lut 620	Inf	Inf	Inf	Inf	Inf	Inf	Inf	Inf	Inf	60.4	489.9	–	Inf	Inf	Inf
Lut 621	Inf	343.7	22.5	89.9	Inf	697.8	750.6	Inf	Inf	Inf	Inf	Inf	–	Inf	Inf
Vio 622	Inf	Inf	Inf	Inf	Inf	Inf	Inf	Inf	Inf	Inf	251.3	Inf	Inf	–	Inf
Neo 623	Inf	Inf	Inf	174.6	Inf	187.3	Inf	288.8	Inf	Inf	Inf	Inf	Inf	Inf	–