

**Supporting Information of the manuscript entitled “Cost-effective Solar Concentrators
based on Red Fluorescent Zn(II)-Salicylaldiminato Complex”, by Pierpaolo Minei,^a**

Elisabetta Fanizza,^{b,c} Antonio M. Rodríguez,^d Ana Belén Muñoz-García,^d Paola Cimino,^e

Michele Pavone,^{d,} Andrea Pucci^{f,g,*}*

^aScuola Normale Superiore, Piazza dei Cavalieri 7, I-56126 Pisa, Italy

^bDipartimento di Chimica, Università degli Studi di Bari, Via Orabona 4, 70126 Bari, Italy

^cCNR-Istituto per i Processi Chimico Fisici, UOS Bari, Via Orabona 4, 70126 Bari, Italy

^dDipartimento di Scienze Chimiche, Università di Napoli Federico II, Complesso Universitario Monte Sant'Angelo Via Cintia 21, 80126 Napoli, Italy

^eDipartimento di Scienze Farmaceutiche Università degli Studi di Salerno, Via Ponte don Melillo, I-84084 Fisciano (Salerno) Italy

^fDipartimento di Chimica e Chimica Industriale, Università di Pisa, Via Moruzzi 13, 56124 Pisa, Italy

^gINSTM, UdR Pisa, Via Moruzzi 13, 56124 Pisa, Italy

The Thorlabs FDS1010 photodiode is ideal for measuring both pulsed and CW light sources, by converting the optical power to an electrical current. The Si detector is mounted on a 0.45”x0.52” ceramic wafer package with an anode and cathode. The photodiode anode produces a current, which is a function of the incident light power and the wavelength (Figure S1)

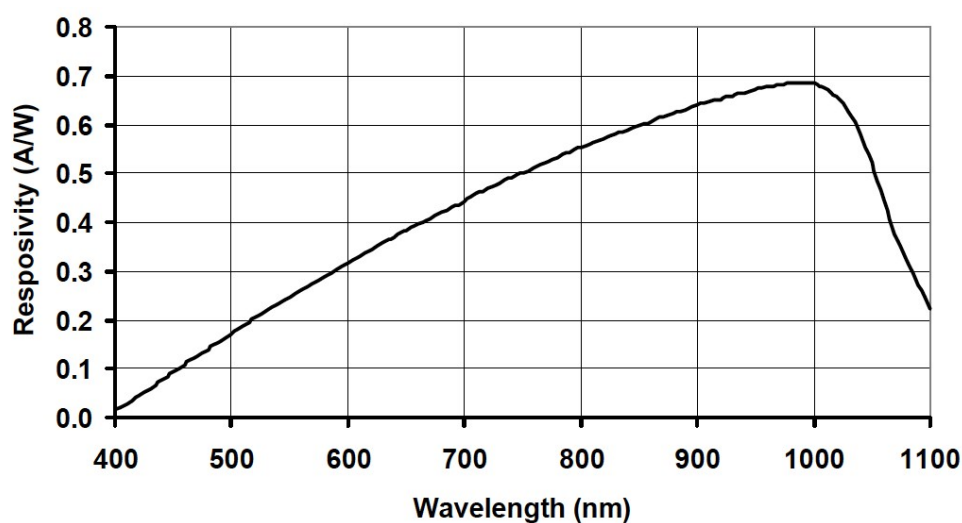


Figure S1. Typical Responsivity curve using Thorlabs calibration services

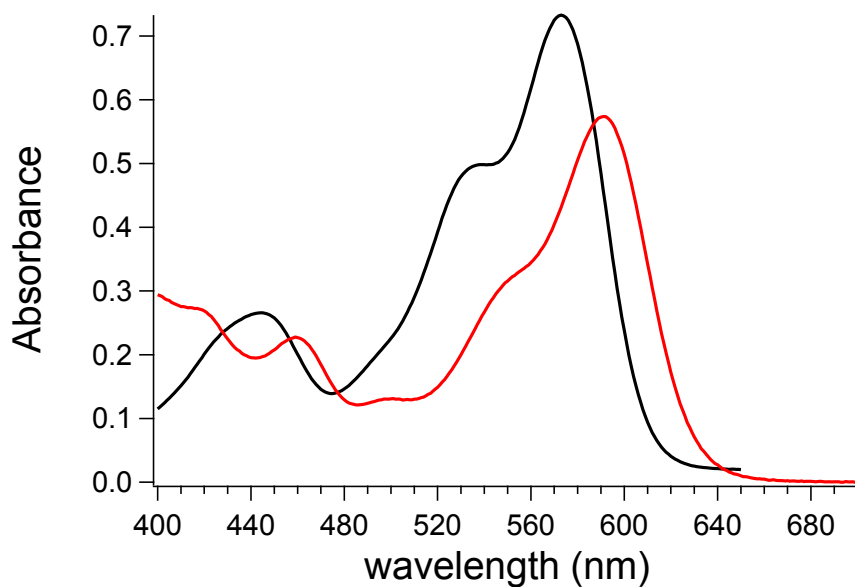


Figure S2. Absorption spectra of PMMA film containing 1% of different dyes: LR (black), *ZnL* (red). For all systems, the film thickness was 25 ± 5 μm .

Table S1. Convergence study of the correct functional for the description of the *ZnL* system in DOX solution, calculations carried out with the LANL2TZ+ and 6-311++G(d,p) basis set.

PCM=DOX			
Entry	λ_{abs} (nm)	λ_{ems} (nm)	Stokes Shift (nm)
B3LYP	549.02	586.58	37.558
CAM-B3LYP	463.17	508.71	45.543
M062x	470.11	517.74	47.624
PBE0	525.26	561.43	36.166

Table S2. Convergence study of the basis set for the description of the Stokes Shift for the *ZnL* gas-phase system. Zn atom is described with LANL2TZ+ ECP and basis set.

B3LYP/(basis set)				
Entry	λ_{abs} (nm)	λ_{ems} (nm)	Stokes Shift (nm)	n. basis func.
6-31G(d)	524.25	556.41	32.16	505
6-31+G(d,p)	535.07	569.14	34.07	675
6-31+G(2d,2p)	534.26	568.47	34.21	877
6-31++G(d,p)	535.07	569.14	34.07	689
6-31++G(2d,2p)	534.29	568.52	34.23	891
6-311G(d,p)	524.8	558.72	33.92	689
6-311++G(d,p)	531.52	566.51	34.99	831
6-311++G(2d,2p)	530.7	565.92	35.22	1033

Table S3. Computed structural and electronic parameters of ground-state (S_0) *ZnL* in DOX and THF solutions: distances in Å, angles and dihedral angles in degrees ($^\circ$), S_0 - S_1 vertical excitation energies (λ_{abs} , in nm) computed on the ground state minima, values inter parenthesis are the relative computed oscillator strength (f).

	DOX		THF	
	<i>ZnL</i>-PCM	<i>ZnL</i>-DOX₂-PCM	<i>ZnL</i>-PCM	<i>ZnL</i>-THF₂-PCM
Zn-N1 (Zn-N1')	2.117 (2.117)	2.151 (2.153)	2.128 (2.128)	2.158 (2.159)
Zn-O (Zn-O')	1.976 (1.976)	2.021 (2.020)	1.989 (1.989)	2.032 (2.032)
N1-C1 (N1'-C1')	1.380 (1.380)	1.379 (1.378)	1.378 (1.378)	1.376 (1.377)
C1-C2	1.427	1.429	1.428	1.429
C2-N2	1.157	1.157	1.157	1.157
O-Zn-N1	87.1	85.9	87.0	85.7
N1-Zn-N1'	79.0	78.2	78.9	78.2
N1-C1-C2	121.1	121.1	121.3	121.4
C1-C2-N2	176.9	176.7	177.6	177.4
N1-C1-C2-N2	0.0	1.0	0.0	0.4
N1-O-O'-N1'	0.0	0.3	0.0	1.1
N1-C3-C-C4	0.0	2.7	0.0	0.3
Zn-solvent	--	2.357	--	2.292
λ_{abs} exp.	589		595	
λ_{abs} TD-DFT	549 (0.886)	573 (0.796)	547 (1.043)	580 (0.990)

Table S4. Computed structural and electronic parameters of excited-state (S_1) *ZnL* in DOX and THF solutions: distances in Å, angles and dihedral angles in degrees (°). Vertical emission energies (λ_{ems} , in nm) computed on the first excited state minima, values inter parenthesis are the relative computed oscillator strength (f), structural deviations from the ground state minima are also reported (Δ_{S0-S1}).

	<i>ZnL</i>-DOX₂-PCM	Δ_{S0-S1}	<i>ZnL</i>-THF₂-PCM	Δ_{S0-S1}
Zn-N1 (Zn-N1')	2.150 (2.158)	-0.001 (0.005)	2.165 (2.165)	0.007 (0.006)
Zn-O (Zn-O')	2.024 (2.027)	0.003 (0.007)	2.036 (2.036)	0.004 (0.004)
N1-C1 (N1'-C1')	1.363 (1.367)	-0.016 (-0.011)	1.359 (1.359)	-0.017 (-0.018)
C1-C2	1.419	-0.010	1.418	-0.011
C2-N2	1.160	0.003	1.161	0.004
O-Zn-N1	86.8	0.9	86.2	0.5
N1-Zn-N1'	79.1	0.9	78.9	0.7
N1-C1-C2	121.1	0.0	121.3	-0.1
C1-C2-N2	176.8	0.1	177.6	0.2
N1-C1-C2-N2	1.9	0.9	0.6	0.2
N1-O-O'-N1'	0.1	-0.2	2.1	1.0
N1-C3-C-C4	2.8	0.1	2.1	1.8
Zn-solvent	2.327	-0.030	2.271	-0.021
λ_{ems} exp.	621	--	630	--
λ_{ems} TD-DFT	615 (0.796)	--	631 (0.989)	--

Table S5. Computed structural and electronic parameters of ground-state (S_0) excited-state (S_1) of ZnL in PMMA, and corresponding structural variations ($\Delta_{S_0-S_1}$): distances in Å, angles and dihedral angles in degrees ($^\circ$). Vertical excitation (λ_{abs}) and emission (λ_{ems}) energies in nm, values inter parenthesis are the corresponding computed oscillator strength (f).

	<i>Ground State</i> <i>ZnL-PMMA₂-PCM</i>	<i>Excited State</i> <i>ZnL-PMMA₂-PCM</i>	$\Delta_{S_0-S_1}$
Zn-N1 (Zn-N1')	2.153 (2.153)	2.162 (2.162)	0.009 (0.009)
Zn-O (Zn-O')	2.021 (2.021)	2.030 (2.030)	0.009 (0.009)
N1-C1 (N1'-C1')	1.377 (1.377)	1.361 (1.360)	-0.016 (-0.017)
C1-C2	1.4	1.4	0.0
C2-N2	1.2	1.2	0.0
O-Zn-N1	85.5	85.8	0.3
N1-Zn-N1'	78.3	79.0	0.7
N1-C1-C2	121.2	121.2	0.0
C1-C2-N2	177.0	177.1	0.1
N1-C1-C2-N2	1.3	2.4	1.1
N1-O-O'-N1'	0.2	1.8	1.5
N1-C3-C-C4	2.5	1.6	-0.9
Zn-solvent	2.350	2.306	-0.044
λ_{abs} TD-DFT	577 (0.767)	--	--
λ_{ems} TD-DFT	--	619 (0.887)	--

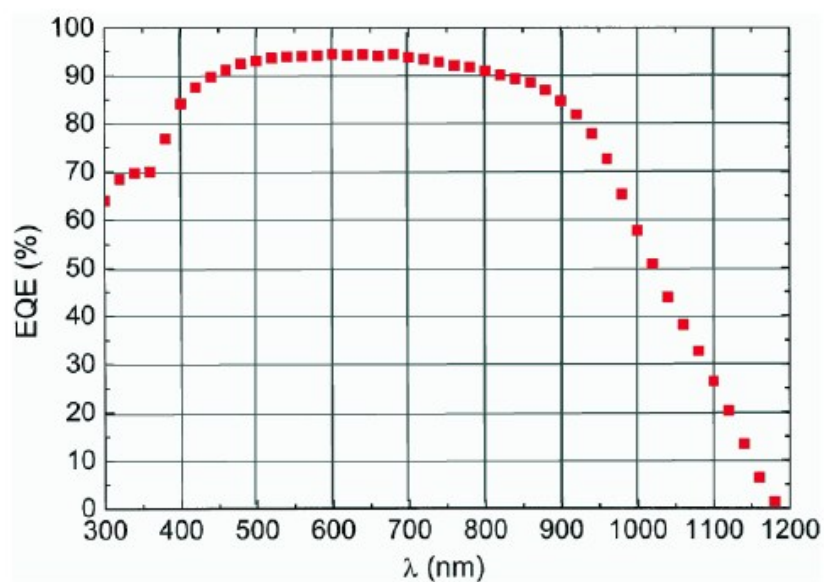


Figure S3. External quantum efficiency of the PV cell