

# ADVANCED MATERIALS

## Supporting Information

for *Adv. Mater.*, DOI: 10.1002/adma.202005940

Conjugated Organic Photothermal Films for  
Spatiotemporal Thermal Engineering

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Eunyoung Kim\**

## Supporting Information

# Conjugated Organic Photothermal Films for Spatiotemporal Thermal Engineering

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Keywords: conjugated polymers, photothermal properties, synthesis, photoacutination, energy harvesting, water evaporation

**Table S1.** Symbols list (alphabetical order)

Symbol	Full name
$a$	surface area
$\nabla T$	temperature gradient
$C_p$	heat capacity
$C_p$	specific heat capacity
$d_{\text{HCS}}$	diameter of harvested cell sheet
$d_{\text{NIR}}$	diameter of NIR- exposed area
$E_F$	Fermi level
$f(E)$	the Fermi–Dirac distribution function
$g_V(E)$	density of state
$H$	enthalpy of liquid- vapor phase change
$h$	heat-transfer coefficient

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$H_e$	heat of evaporation of the water
$I$	output current
$I_{pd}$	(light) power density
$l$	thickness
$m$	mass
$m_w$	mass of evaporated water
$p$	carrier concentration
$P$	output power
$p_0$	initial pressure rise
$PF_{PTE}$	PTE power factor
$Q_{cond}$	heat conduction
$Q_{conv}$	heat convection
$Q_e$	power density for evaporation of water
$Q_i$	incident light power density
$Q_{PT}$	heat for a photothermal effect
$Q_{rad}$	heat radiation
$Q_{surr}$	heat loss to the surrounding environment
$R$	resistance between the two electrodes
$S_{PTE}$	photothermoelectric Seebeck coefficient
$S_{TE}$	thermoelectric Seebeck coefficient
$T$	temperature
$T_{max}$	maximum temperature
$T_{surr}$	surrounding temperature of system
$V$	output voltage
$\beta$	isobaric volume expansion coefficient
$\Gamma$	Grüneisen parameter
$\Delta T$	temperature difference
$\Delta T_{PT}$	temperature increase by photothermal effect
$\Delta v$	difference in evaporation rates with and without light
$\varepsilon$	absorption coefficient
$\eta_d$	efficiency of cell detachment
$\eta_{PT}$	photothermal conversion efficiency
$\eta_{PTE}$	photothermoelectric efficiency
$\eta_{PTW}$	photothermal efficiency of water vaporization
$\eta_{STE}$	solar thermal efficiency
$\eta_w$	water evaporation efficiency
$\theta$	dimensionless temperature ratio
$\theta_b$	bending angle
$\kappa$	isothermal compressibility
$\lambda_{abs}$	maximum absorption wavelength
$\lambda_{PT}$	light wavelength for PT engineering
$\mu$	carrier (Hall) mobility
$\mu_a$	absorption coefficient of tissue
$\rho$	mass density
$\sigma_e$	electrical conductivity
$\tau_s$	time constant

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**Table S2.** Abbreviations list (alphabetical order)

Abbreviation	Full name
A	acceptor
ADSC	adipose- derived stem cell
AM	antimicrobial
APTES	(3-aminopropyl)triethoxysilane
AVT	average visible transmittance
f-BNNS	functionalized boron nitrogen nanosheet
BSM	black sesame melanin
BT	benzothiadiazole
CP	conjugated polymer
CPM	constant potential method
Croc	croconaine
Croc-c	2,5-bis[(4-carboxylic-piperidylamino)thiophenyl]-croconium
CS	cell sheet
CTE	coefficient of thermal expansion
CTGS	carbonized towel- gourd sponges
CV	cyclic voltammogram
CVD	chemical vapor deposition
Cy	cyanine
D	donor
DCB	1,2-dichlorobenzene
DCM	dichloromethane
DI	diimmonium salt
DMF	dimethylformamide
DOS	density of state
DOX	doxorubicin hydrochloride
DPP	diketopyrrolopyrrole
DPPT	poly{2,2'-[(2,5-bis(2-hexyldecyl)-3,6-dioxo-2,3,5,6-tetrahydropyrrolo[3,4-c]pyrrole-1,4-diyl)dithiophene]-5,5'-diyl- <i>alt</i> -thiophene-2,5-diyl}
DPPV	poly{2,2'-[(2,5-bis(2-hexyldecyl)-3,6-dioxo-2,3,5,6-tetrahydropyrrolo[3,4-c]pyrrole-1,4-diyl)dithiophene]-5,5'-diyl- <i>alt</i> -vinyle
DSPE-PEG2000	1,2-distearoyl- <i>sn</i> -glycero-3-phosphoethanolamine- <i>N</i> -[methoxy(polyethylene glycerol)-2000]
DSSC	dye-sensitized solar cell
DT	2,2'-bithiophene
DTP	4H-dithieno[3,2- <i>b</i> :2',3'- <i>d</i> ]pyrrole
EB	emeraldine base
EDOT	3,4-ethylenedioxythiophene
ES	emeraldine salt
EXIM	excited-state intramolecular motion

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FDA	the U.S. Food and Drug Administration
FESEM	field emission scanning electron microscopy
FL	fluorescence
FLI	fluorescence imaging
GO	graphene oxide
ICG	indocyanine green
ICT	intramolecular charge transfer
IDI	isobutyl-substituted diimmonium borate
IPA	<i>N,N,N',N'</i> - tetrakis[4- (diisobutylamino)phenyl]- 1,4-phenylenediamine
IR-780	2-[2-[2-chloro-3-[(1,3-dihydro-3,3-dimethyl-1-propyl-2H-indol-2-ylidene)ethylidene]-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-1-propylindolium iodide
IR-820	2-[2-[2-chloro-3-[[1,3-dihydro-1,1-dimethyl-3-(4-sulfobutyl)-2H-benzo[e]indol-2-ylidene]-ethylidene]-1-cyclohexen-1-yl]-ethenyl]-1,1-dimethyl-3-(4-sulfobutyl)-1H-benzo[e]indolium hydroxide inner salt
IR-825	3-(4-carboxybenzyl)-2-((E)-2-((E)-3-((Z)-2-(3-(4-carboxybenzyl)-1,1-dimethyl-1,3-dihydro-2H-benzo[e]indol-2-ylidene)ethylidene)-2-chlorocyclohex-1-en-1-yl)vinyl)-1,1-dimethyl-1H-benzo[e]indol-3-ium bromide
ISC	intersystem crossing
ITO	indium tin oxide
LC	liquid crystal
LED	light emitting diode
mol-PT	molecular photothermal
Molecule (1)	1,1,2-trimethyl-1H-benzo[e]indole
Molecule (2)	4-(1,1,2-trimethyl-1H-benzo[e]indolium-3-yl)butane-1-sulfonate
Molecule (3)	<i>N</i> -phenyl- <i>N</i> -((1 <i>E</i> ,3 <i>E</i> ,5 <i>E</i> )-5-(phenylimino)penta-1,3-dienyl)acetamide triethyl amine
Monomer (4)	3,6-bis(5-bromothiophene-2-yl)-2,5-bis(2-hexyldecyl)pyrrolo[3,4- <i>c</i> ]pyrrole-1,4-(2 <i>H</i> ,5 <i>H</i> )-dione
Monomer (5)	<i>trans</i> -1,2-bis(tributylstannyl)ethene
Monomer (6)	dibromo-thiophene-fused benzodifurandione-based oligo( <i>p</i> -phenylenevinylene)
Monomer (7)	2-(trimethylstannyl)-5-(5-(trimethylstannyl)thiophen-2-yl)thiophene
Monomer (8)	terephthalonitrile
Monomer (9)	2,5-diaminobenzene-1,4-dithiol
MW	microwave
MXene	Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> , where T is a functional group (e.g. O, F, OH, Cl)
NIR	near infrared
NP	nanoparticle
NRD	nonradiative decay
P3HT	poly(3-hexylthiophene)
PANI	polyaniline

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PA	photoacoustic
PAI	photoacoustic imaging
PAT	photoacoustic therapy
PATo	photoacoustic tomography
PCE	photothermal conversion efficiency
PCL	polycaprolactone
PCPDTBSe	poly[4,4-bis(2-ethylhexyl)-cyclopenta[2,1-b;3,4-b']dithiophene-2,6-diyl- <i>alt</i> -2,1,3-benzoselenadiazole-4,7-diyl]
PCPDTBT	poly[2,6-(4,4-bis-(2-ethylhexyl)-4H-cyclopenta[2,1-b;3,4-b']dithiophene)- <i>alt</i> -4,7(2,1,3-benzothiadiazole)]
PDA	polydopamine
PDMS	poly(dimethylsiloxane)
PDPPTDQ	poly{2,2'-[(2,5-bis(2-ethylhexyl)-3,6-dioxo-2,3,5,6-tetrahydropyrrolo[3,4-c]pyrrole-1,4-diyl)dithiophene]-5,5'-diyl- <i>alt</i> -[6,7(4-hexylphenyl)-[1,2,5]thiadiazolo[3,4-g]quinoxaline]}
PDPPTTh	poly[diketopyrrolopyrrole- <i>alt</i> -thiophene]
PDPTBT	poly(7-pentadecane-4H-dithieno[3,2-b:2',3'-d]pyrrole- <i>alt</i> -2,1,3-benzothiadiazole)
PDPTDPP	poly[7-pentadecane-4H-dithieno[3,2-b:2',3'-d]pyrrole- <i>alt</i> -2,5-bis(2-octylododecyl)-3,6-di(thiophen-2-yl)pyrrolo[3,4-c]pyrrole-1,4(2H,5H)-dione]
PDPTPT	poly(7-pentadecane-4H-dithieno[3,2-b:2',3'-d]pyrrole- <i>alt</i> -1,2,5-thiadiazolo[3,4-c]pyridine)
PDT	photodynamic therapy
PE	piezoelectric
PEDOS	poly(3,4-ethylenedioxy-selenophene)
PEDOS-C6	hexyl-derivatized poly(3,4-ethylenedioxy-selenophene)
PEDOT	poly(3,4-ethylenedioxythiophene)
PEDOT-S	propane-1-sulfonated poly(3,4-ethylenedioxythiophene)
PEDOT:PSS	polystyrene sulfonate doped poly(3,4-ethylenedioxythiophene)
PEPG	poly(ethylene glycol)- <i>block</i> -poly(propylene glycol)- <i>block</i> -poly(ethylene glycol)
PES	polyethersulfone
PET	polyethylene terephthalate
PETo	positron emission tomography
PF	NIR-blocking plastic filter
PFBT	poly(9,9-dihexylfluorene- <i>alt</i> -2,1,3-benzothiadiazole)
PFTTQ	poly[9,9-bis(4-(2-ethylhexyl)phenyl)-fluorene- <i>alt-co</i> -6,7-bis(4-(hexyloxy)phenyl)-4,9-di-(thiophen-2-yl)thiadiazoloquinoxaline]
PM	photo-mechanical
PMMA	poly(methyl methacrylate)
PNIPAM	poly(N-isopropylacrylamide)
pol-PT	polymeric photothermal
Poly[Cu <sub>x</sub> (Cu-ett)]	poly[Cu <sub>x</sub> (Cu-ethylenetetrathiolate)]

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Poly(EDOT-HQ-co-EDOT-PC)	hydroquinone and phosphorylcholine functionalized PEDOT copolymer	
PorCP	porphyrin-based conjugated polymer	
PorCP2	poly([(5,15- diethynyl- 10,20- bis(3,5- bis(octyloxy)phenyl) porphyrinato]zinc- alt- (2,1,3- benzothiadiazole))	
PPBBT	poly(2-phenyl-benzobisthiazole)	
PProDOS	poly(3,4-propylenedioxy-selenophene)	
PPy	polypyrrole	
PS	polystyrene	
PT	photothermal	
PTA	photothermal actuator	
PTCS	photothermal cell sheet harvesting	
PTE	photothermoelectric	
PTH	photothermal heater	
PTHC	photothermal harvesting of cells	
PTII	poly(thienoisindigo)	
PTSC	photothermal single cell harvesting	
PTT	photothermal therapy	
PTW	photothermal water evaporation	
PU	polyurethane	
PV	photovoltaic	
PVA	polyvinyl alcohol	
PVDF	poly(vinylidene fluoride)	
PVDF-TrFE	poly(vinylidene fluoride- <i>co</i> -trifluoroethylene)	
PVPS	poly(vinylpyrrolidone) sulfobetaine	
RGO	reduced graphene oxide	
ROS	releases singlet oxygen	
SC	single cell	
SCP	solution casting polymerization	
SE	Stirling engine	
SEM	scanning electron microscopy	
SPR	surface plasmon resonance	
SS	stainless steel	
STE	solar thermal efficiency	
TBDOPV	thiophene-fused benzodifurandione-based phenylenevinylene)	oligo(p-
TBDOPV-DT	thiophene-fused benzodifurandione-based phenylenevinylene)-2,2'-bithiophene	oligo(p-
TE	thermoelectric	
Tos	tosylate	
TzQI-TDPP	poly(thiadiazoloquinoxalinimide-thiophene-flanked diketopyrrolopyrrole)	
UV	ultraviolet	

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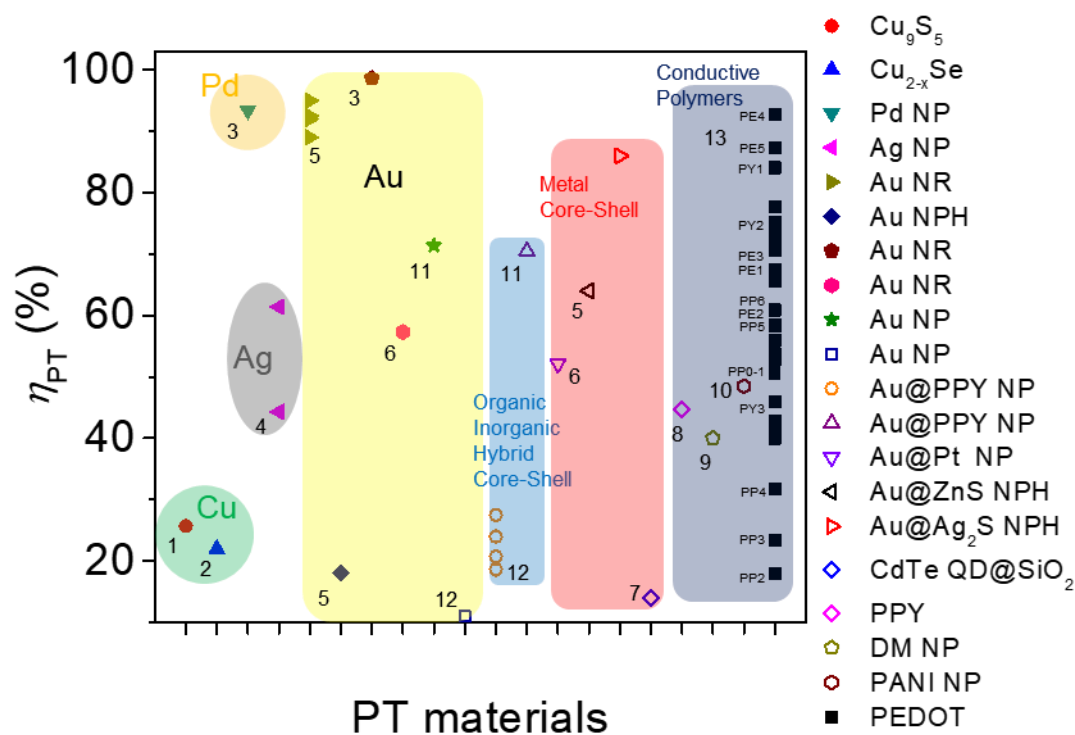


Figure S1. Photothermal conversion efficiency of various photothermal materials including metals, conductive polymers, and organic-inorganic hybrid materials. NP: nanoparticle, NR: nanorod, NPH: nanopolyhedron, PPY: polypyrrole, QD: quantum dot, DM: dopamine melanin, PANI: polyaniline. The number near the data point is the reference number of the sample.<sup>[1-13]</sup>

## References

- [1] Q. Tian, F. Jiang, R. Zou, Q. Liu, Z. Chen, M. Zhu, S. Yang, J. Wang, J. Wang, J. Hu, *ACS Nano* **2011**, 5, 9761.
- [2] C. M. Hessel, V. P. Pattani, M. Rasch, M. G. Panthani, B. Koo, J. W. Tunnell, B. A. Korgel, *Nano Lett.* **2011**, 11, 2560.



- [3] J.-W. Xiao, S.-X. Fan, F. Wang, L.-D. Sun, X.-Y. Zheng, C.-H. Yan, *Nanoscale* **2014**, 6, 4345.
- [4] D. Wen, H. Zhang, H.-J. Chen, G. Lin, *4th Micro and Nano Flows Conference* **2014**, 1.
- [5] H. Chen, L. Shao, T. Ming, Z. Sun, C. Zhao, B. Yang, J. Wang, *Small* **2010**, 6, 2272.
- [6] J. Tang, X. Jiang, L. Wang, H. Zhang, Z. Hu, Y. Liu, X. Wu, C. Chen, *Nanoscale* **2014**, 6, 3670.
- [7] M. Chu, X. Pan, D. Zhang, Q. Wu, J. Peng, W. Hai, *Biomaterials* **2012**, 33, 7071.
- [8] M. Chen, X. Fang, S. Tang, N. Zheng, *Chem. Commun.* **2012**, 48, 8934.
- [9] Y. Liu, K. Ai, J. Liu, M. Deng, Y. He, L. Lu, *Adv. Mater.* **2013**, 25, 1353.
- [10] J. Zhou, Z. Lu, X. Zhu, X. Wang, Y. Liao, Z. Ma, F. Li, *Biomaterials* **2013**, 34, 9584.
- [11] M. Lin, C. Guo, J. Li, D. Zhou, K. Liu, X. Zhang, T. Xu, H. Zhang, L. Wang, B. Yang, *ACS Appl. Mater. Interfaces* **2014**, 6, 5860.
- [12] J. Li, J. Han, T. Xu, C. Guo, X. Bu, H. Zhang, L. Wang, H. Sun, B. Yang, *Langmuir* **2013**, 29, 7102.
- [13] B. Kim, M. Han, E. Kim, *J. Mater. Chem. A* **2019**, 7, 2066.