Science Advances
AAAS

advances.sciencemag.org/cgi/content/full/6/21/eaaz6107/DC1

Supplementary Materials for

Large-scale preparation for efficient polymer-based room-temperature phosphorescence via click chemistry

R. Tian, S.-M. Xu, Q. Xu, C. Lu*

*Corresponding author. Email: luchao@mail.buct.edu.cn

Published 20 May 2020, *Sci. Adv.* **6**, eaaz6107 (2020)
DOI: 10.1126/sciadv.aaz6107

This PDF file includes:

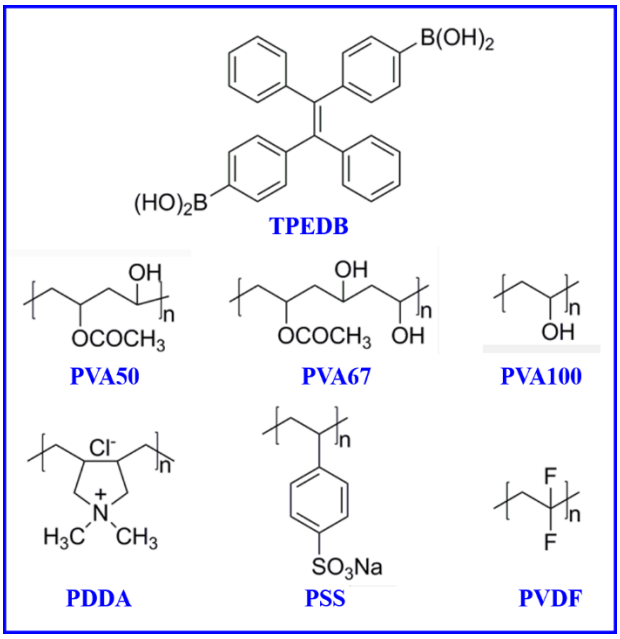

Fig. S1. Molecular formulae of phosphors and polymer matrices. The molecular formulae of TPEDB, PVA with different alcoholysis degree (PVA50, PVA67, PVA100), and controlled polymers (PDDA, PSS, and PVDF).

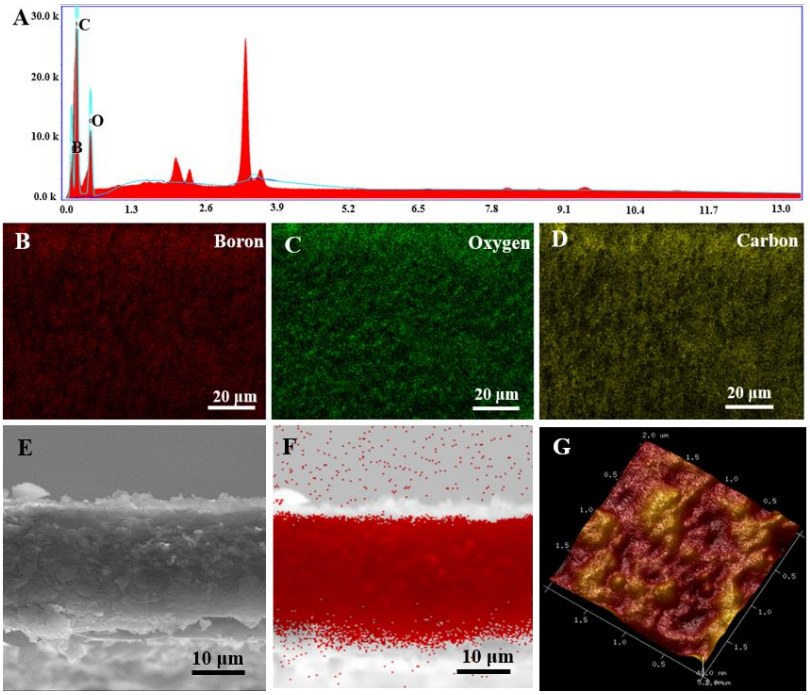

Fig. S2. Morphological studies of TPEDB-PVA polymeric material. (**A**) Element analysis, top-view EDX mapping of (**B**) boron, (**C**) oxygen and (**D**) carbon elements; (**E**) side-view image, (**F**) merged element distribution for the TPEDB-PVA polymeric material and (**G**) surface observation by the tapping mode of atomic force microscopy.

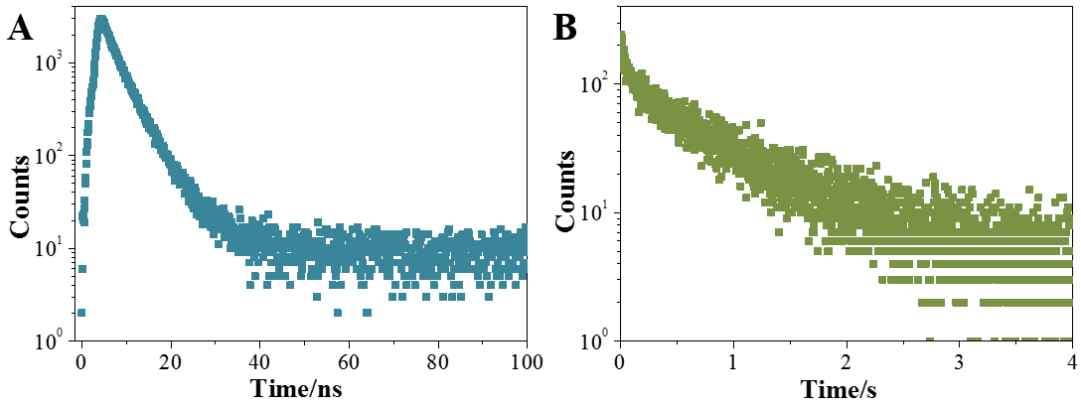

Fig. S3. Luminescent decay curves of TPEDB-PVA polymeric material. (**A**) Fluorescence and (**B**) phosphorescence decay curves of TPEDB-PVA polymeric material with the content of TPEDB of 0.08 mg.

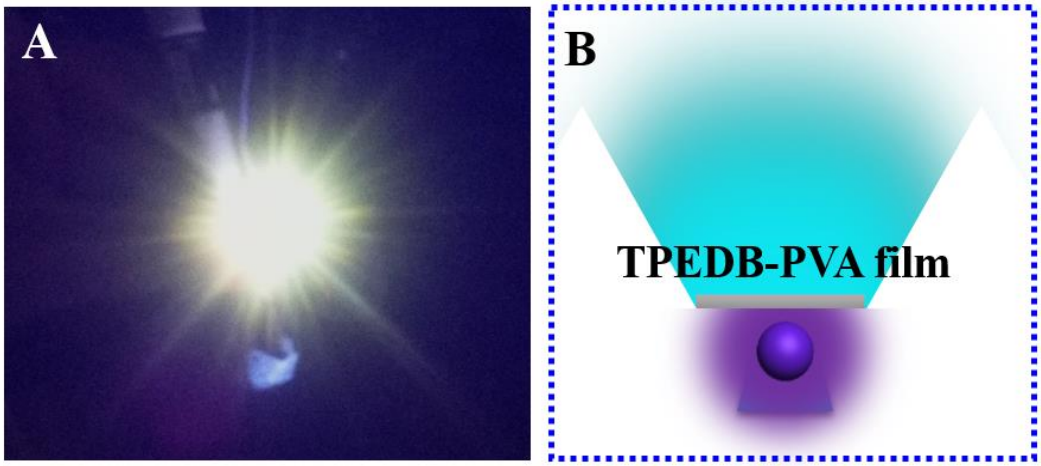

Fig. S4. Schematic illustration for the assembly on LED. (**A**) Photograph of commercial ultraviolet light-emitting diode (UV-LED) and (**B**) schematic illustration of photos for the TPEDB-PVA polymeric material on the UV-LED. Fig. S4A, Photo credit: Qi Xu (coauthor), Beijing University of Chemical Technology.

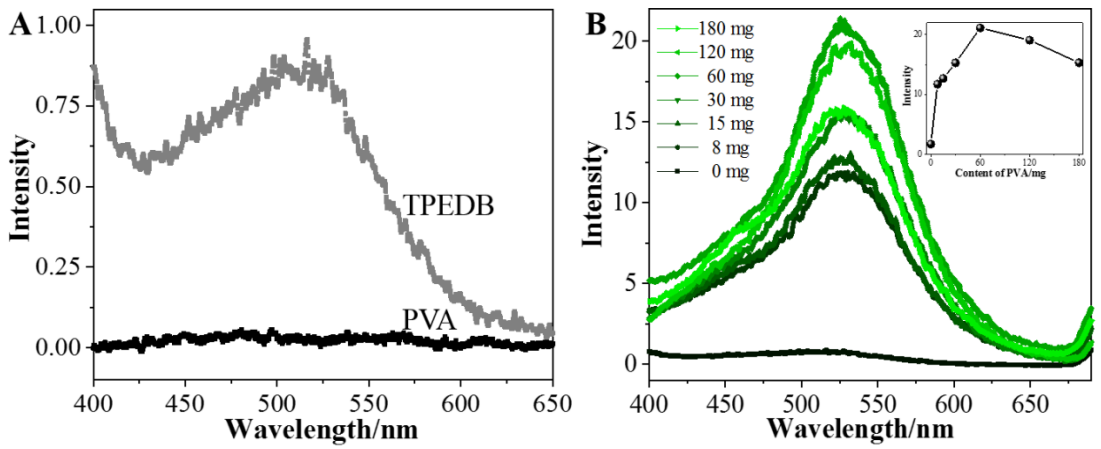

Fig. S5. RTP spectra of TPEDB-PVA polymeric materials. RTP properties of (**A**) TPEDB and PVA, and (**B**) TPEDB-PVA polymeric materials with PVA contents varying from 0 mg to 180 mg; the inset showed the RTP intensity varying with PVA contents.

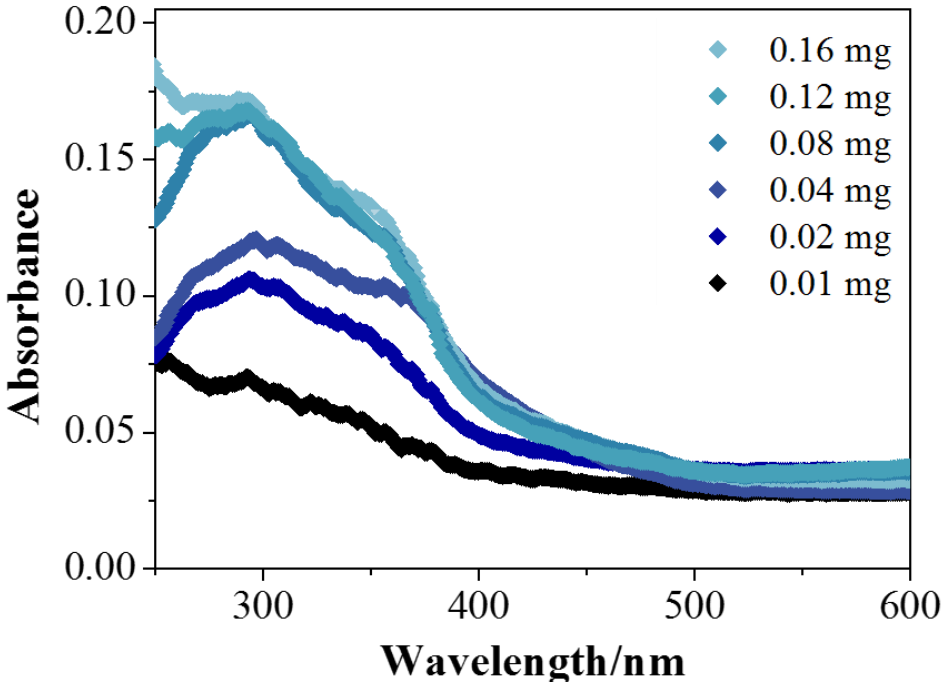

Fig. S6. UV-Vis absorption spectra of TPEDB-PVA polymeric materials. The contents of TPEDB ranged from 0.01 mg, 0.02 mg, 0.04 mg, 0.08 mg, 0.12 mg to 0.16mg, respectively.

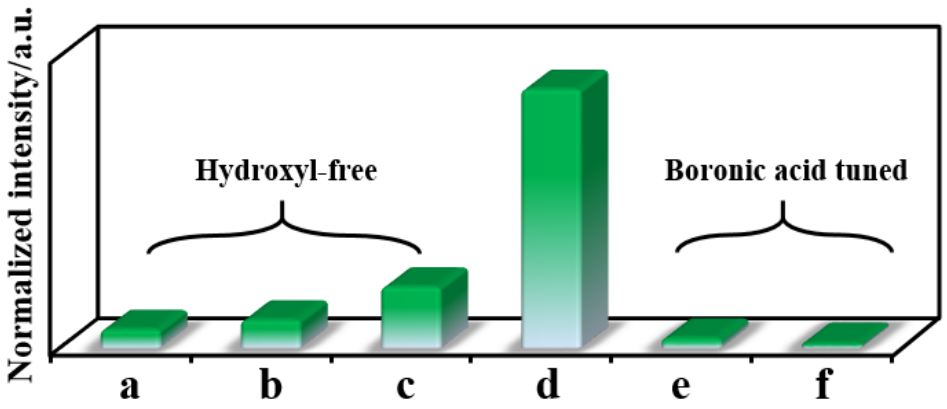

Fig. S7. **RTP intensities of controlled samples**. (**a**) TPEDB-PVDF, (**b**) TPEDB-PSS, (**c**) TPEDB-PDDA, (**d**) TPEDB-PVA, (**e**) TPE-PVA, and (**f**) TPEMB-PVA polymeric materials.

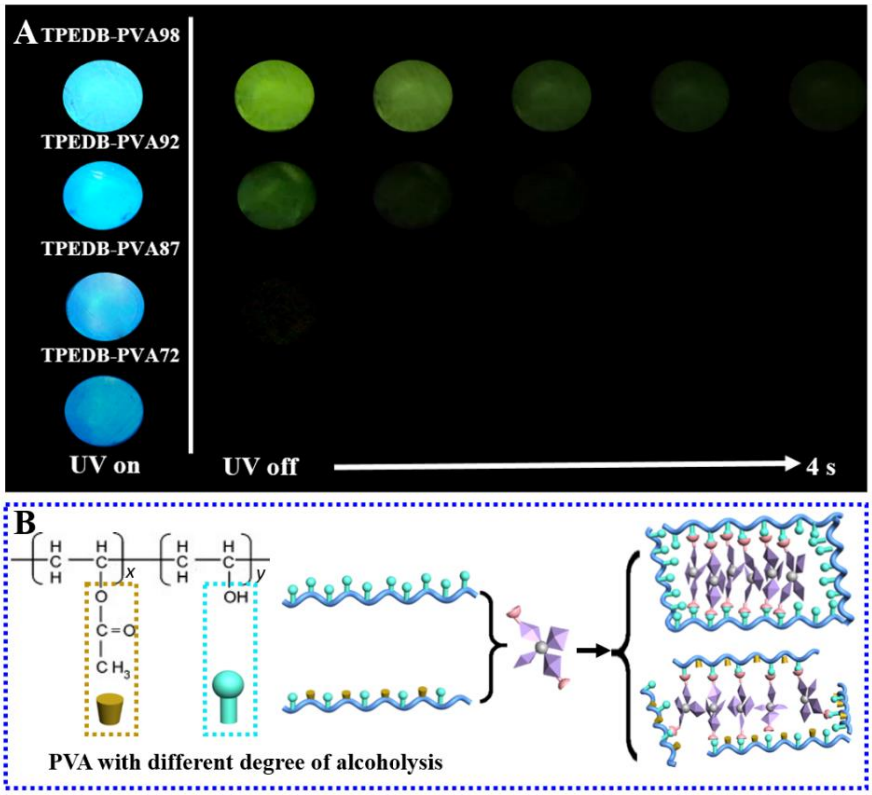

Fig. S8. Luminescent behaviors of TPEDB-PVA polymeric materials. (**A**) Digital photographs of TPEDB-PVA polymeric materials (TPEDB of 0.08 mg) under 365 nm UV irradiation and at different time intervals after removal of UV irradiation, the alcoholysis degree of PVA varied from 72%, 87%, 92%, to 98%; (**B**) schematic representation of the molecular alignment in the TPEDB-PVA polymeric material with different alcoholysis degree of PVA. Fig. S8A, Photo credit: Qi Xu (coauthor), Beijing University of Chemical Technology.

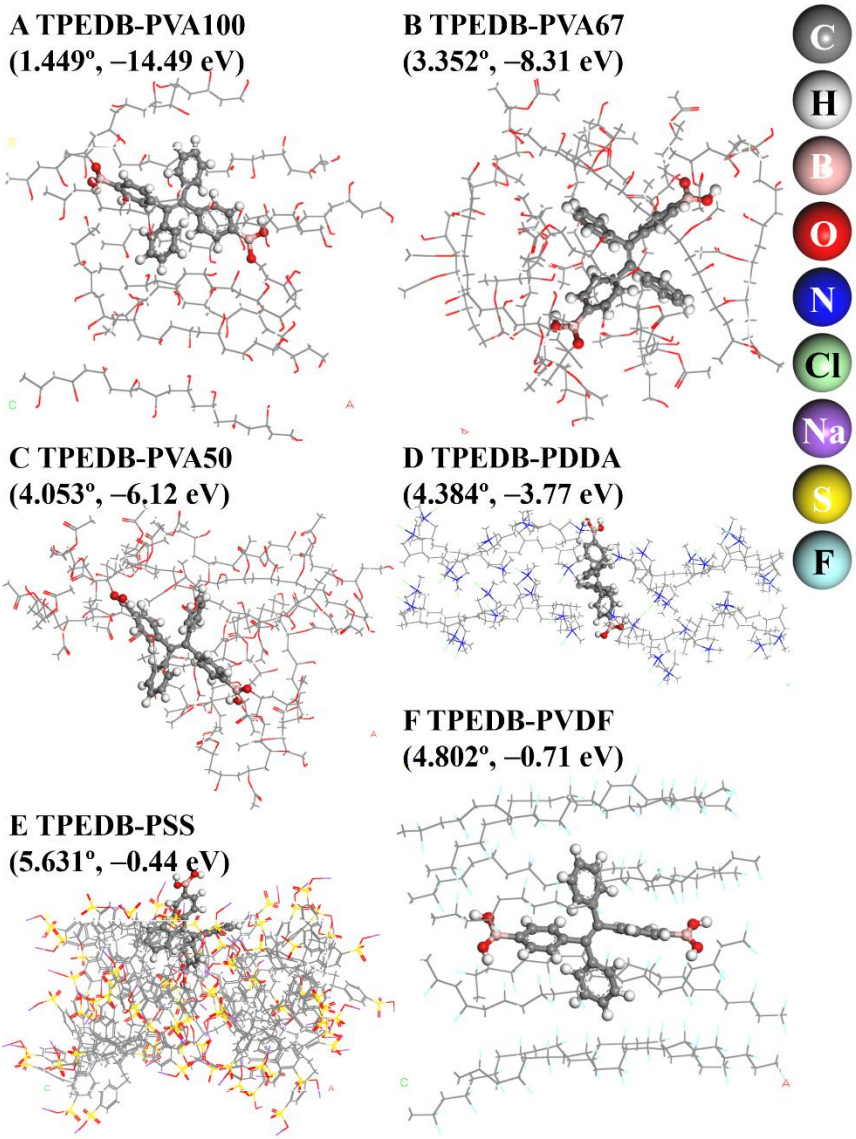

Fig. S9. **Geometrical studies of TPEDB and TPEDB-polymer materials.** (**A**) TPEDB, (**B**) TPEDB-PVA50, (**C**) TPEDB-PVA67, (**D**) TPEDB-PVA100, (**E**) TPEDB-PDDA, (**F**) TPEDB-PVDF, and (**G**) TPEDB-PSS models at the simulation time of 20 ps. The color for each element is labeled. The integral of the dihedral angle away from the equlibrium state ($\sum P\left|d-\overline{d}\right|$) and binding energy (EB) are listed in the bracket.

Table S1. **Descartes coordinates of TPEDB (ground state).**

element	coordinates			element	coordinates		
	x / Å	*y* / Å	*z* / Å		*x* / Å	*y* / Å	*z* / Å
C	–0.4095	–0.5473	0.1014	C	0.3290	2.9576	–0.6366
C	0.4096	0.5473	0.1015	H	1.8649	–0.8767	–1.7239
H	–4.2928	0.9954	–1.9605	C	1.8964	0.4431	–0.0231
C	–4.7310	–0.3035	–0.2801	C	2.7404	1.1642	0.8431
C	–4.1254	–1.0869	0.7222	H	2.3015	1.7834	1.6139
H	–4.7586	–1.6390	1.4032	C	4.1255	1.0873	0.7219
C	–2.7403	–1.1638	0.8434	H	4.7586	1.6396	1.4027
H	–2.3014	–1.7828	1.6144	C	4.7311	0.3036	–0.2801
C	–1.8963	–0.4431	–0.0231	C	3.8792	–0.3946	–1.1569
C	–2.4932	0.3302	–1.0350	H	4.2929	–0.9960	–1.9600
H	–1.8649	0.8763	–1.7242	C	2.4933	–0.3304	–1.0348
C	–3.8791	0.3944	–1.1572	B	–6.2817	–0.2409	–0.3911
H	–0.2064	–5.0291	–1.1939	B	6.2817	0.2409	–0.3910
C	–0.3290	–2.9576	–0.6367	O	–6.9759	0.5710	–1.2697
H	–1.0356	–2.7131	–1.4185	O	–7.0371	–1.0383	0.4359
C	0.1103	–1.9446	0.2360	O	6.9760	–0.5704	–1.2702
C	1.0066	–2.2926	1.2624	O	7.0372	1.0377	0.4365
H	1.3404	–1.5313	1.9533	H	–6.5067	1.1752	–1.8575
C	1.4635	–3.6039	1.3996	H	–7.9999	–0.9768	0.3540
H	2.1490	–3.8512	2.1995	H	6.5069	–1.1740	–1.8587
C	1.0350	–4.5954	0.5126	H	8.0000	0.9762	0.3545
H	1.3901	–5.6119	0.6189	H	–1.3905	5.6117	0.6188
C	0.1359	–4.2668	–0.5062	C	–1.4638	3.6038	1.3995
H	1.0358	2.7132	–1.4183	H	–2.1495	3.8510	2.1993
C	–0.1360	4.2668	–0.5061	C	–1.0067	2.2924	1.2624
H	0.2063	5.0291	–1.1938	H	–1.3405	1.5311	1.9533
C	–1.0353	4.5952	0.5126	C	–0.1103	1.9446	0.2361