Supplementary Information (SI) for Journal of Materials Chemistry A.

Flexoelectricity-enhanced photovoltaic effect in Flexible $LiNbO_3$ nanorod array/PVDF nanocomposites

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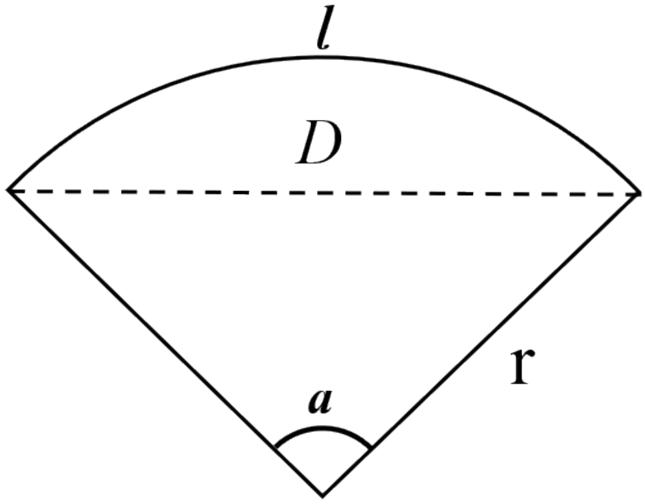
Curvature calculation:



A schematic of the curvature calculation method for the bending film is shown above, where the arc length is defined as *l*; the chord length is defined as D; the radius of curvature is defined as r; the central angle is defined as α. In this investigation, the chord length was measured by the initial and final position of the sliding platform, respectively. Then, the calculation process of curvature (k) in the bending process was calculated as below:

$$2r\sin\frac{\alpha}{2} = D \qquad (Eq.S1)$$

According to the above equations, the central angle (a), radius of curvature (r) and curvature (k=1/r) was calculated as below.

$$r\alpha = l \qquad (Eq.S2)$$

Bandgap Calculation

The linear relationship between $(\alpha h\nu)^2$ and hν is defined using the Tauc formula as below

$$(\alpha hv)^2 = A(hv - E_g) \qquad (Eq.S3)$$

where α, hν, A and E_g is the absorption coefficient, photon energy, a constant and the value of band gap. The calculated band gap of the LN-NR/PVDF-91 nanocomposite is 2.98 eV based on the UV-vis-NIR spectra of the sample.

Table S1. Parameters of the LN-NR/PVDF-91 nanocomposites used in this investigation, including central angle (*a*), radius of curvature (r) and curvature (k=1/r).

Radius (cm)	The sample length (cm)	Film thickness (μm)	The central angel *a*(°)	k(1/m)
5	2	60	22.92	20
6	2	60	19.08	16.67
7	2	60	16.37	14.29
8	2	60	14.32	12.5

Figure S1. SEM images of LN nanosheets (LN-NS) at different scales.

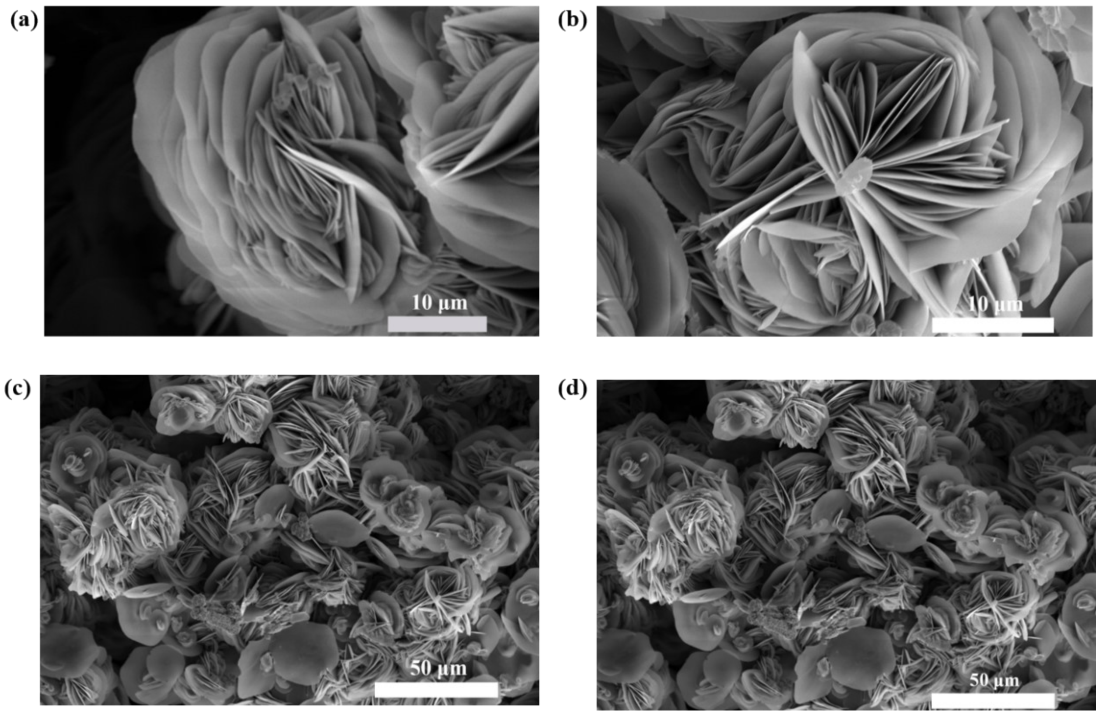


Figure S2. (a) Phase and strain amplitude hysteresis loop vs. applied voltage of the $LiNbO_3$ nanorod (LN-NR) arrays before mixing with the PVDF solution, which was measured using piezoresponse force microscopy (PFM) before they were mixed with PVDF solution.

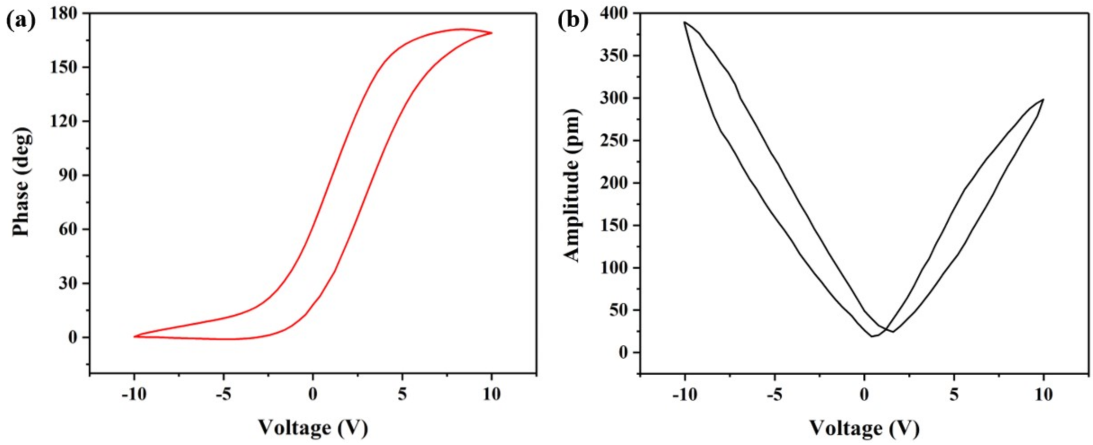


Figure S3. Thermogravimetric analysis (TGA) curves of the LN-NR/PVDF nanocomposites with different $LiNbO_3$ concentrations (heating rate: 10 ℃/min), including 91%, 67% and 36%.

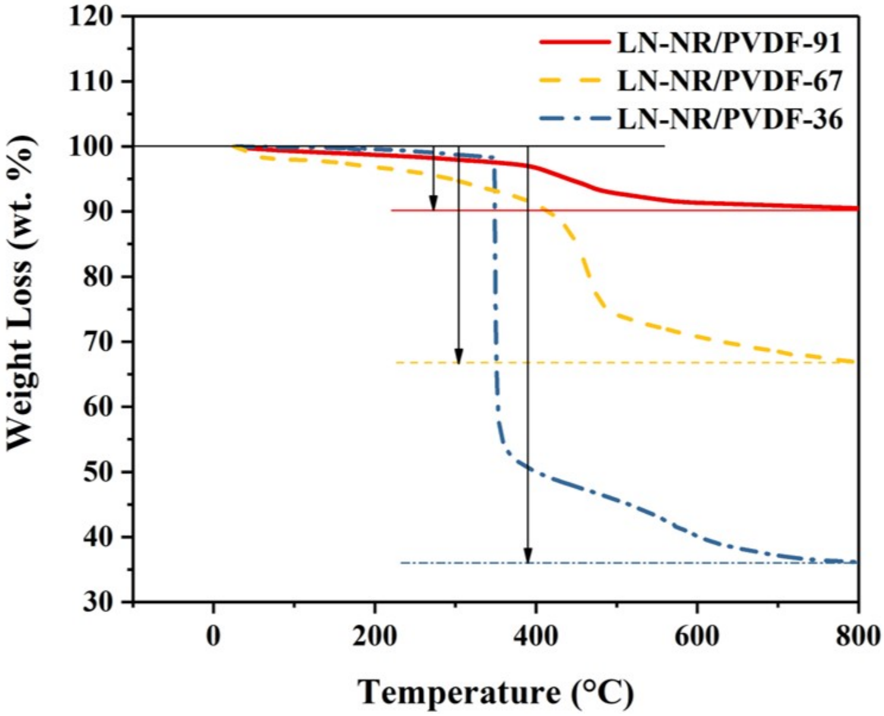


Figure S4. Ultraviolet-Visible-Near Infrared (UV-VIS-NIR) absorption spectra of (a) pristine PVDF film, (c) LN-NR/PVDF-36, (e) LN-NR/PVDF-67, (g) LN-NR/PVDF-91 nanocomposites; the calculated $(\alpha h\gamma)^2$ using Tauc Formula for (b) pristine PVDF film, (d) LN-NR/PVDF-36, (f) LN-NR/PVDF-67, (h) LN-NR/PVDF-91 nanocomposites.

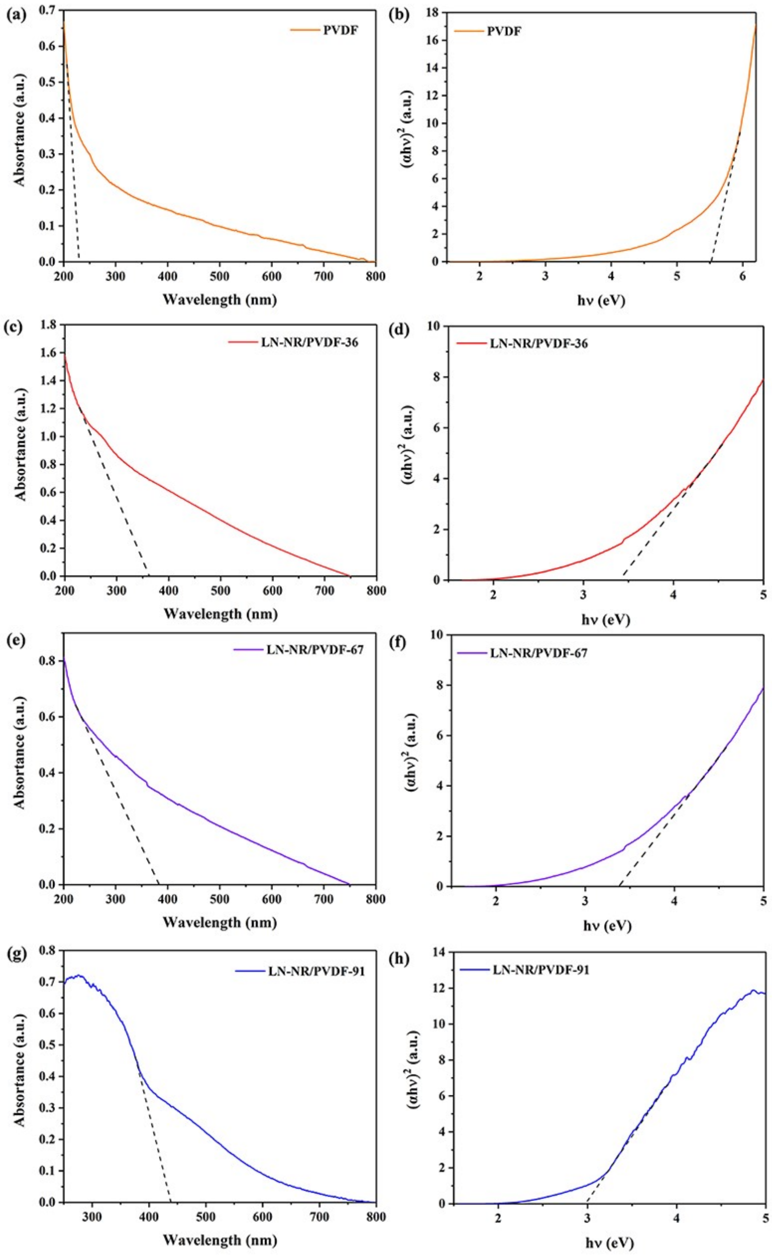


Figure S5. Polarization direction dependence of the PV current (I_{pv}) of the LN-NR/PVDF -91 nanocomposite at a curvature of 1/4, which was measured using a laser (360 nm, 20 mW) with a linear polarizer.

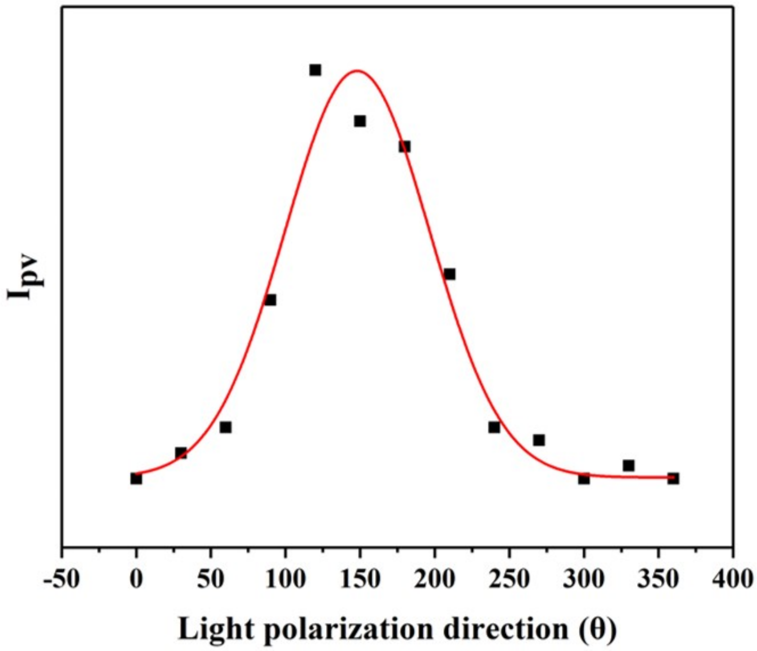


Figure S6. Photovoltaic current (I_{pv}) as a function of curvature (downward bending) of (a) LN-NS/PVDF-67 (LN-nanosheet/PVDF) and (b) LN-NP/PVDF -67 (LN-nanoparticle/PVDF), and I_{pv} as a function of curvature (upward bending) of (c) LN-NS/PVDF-67 and (d) LN-NP/PVDF-67.

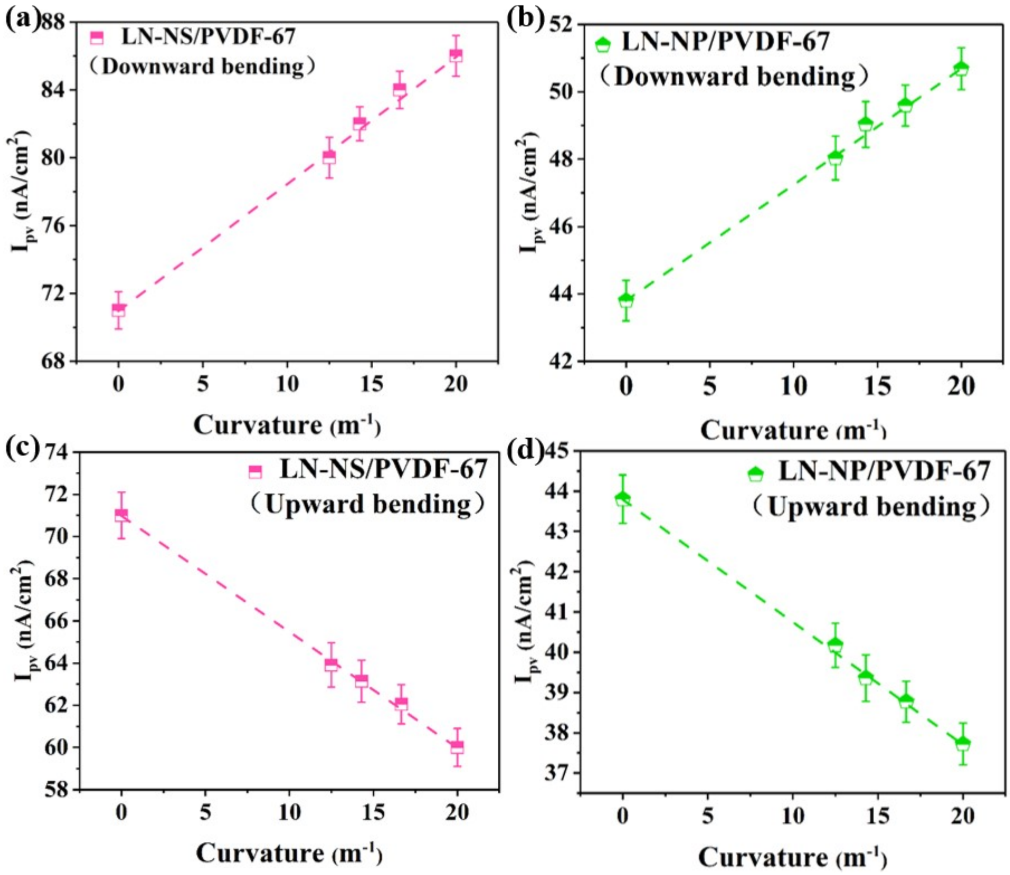


Figure S7. Dielectric constant and dielectric loss of (a) pristine PVDF, (b) LN-NR/PVDF-36, (c) LN-NP/PVDF-67, (d) LN-NS/PVDF-67, (e) LN-NR/PVDF-67, and LN-NR/PVDF-91 nanocomposites.

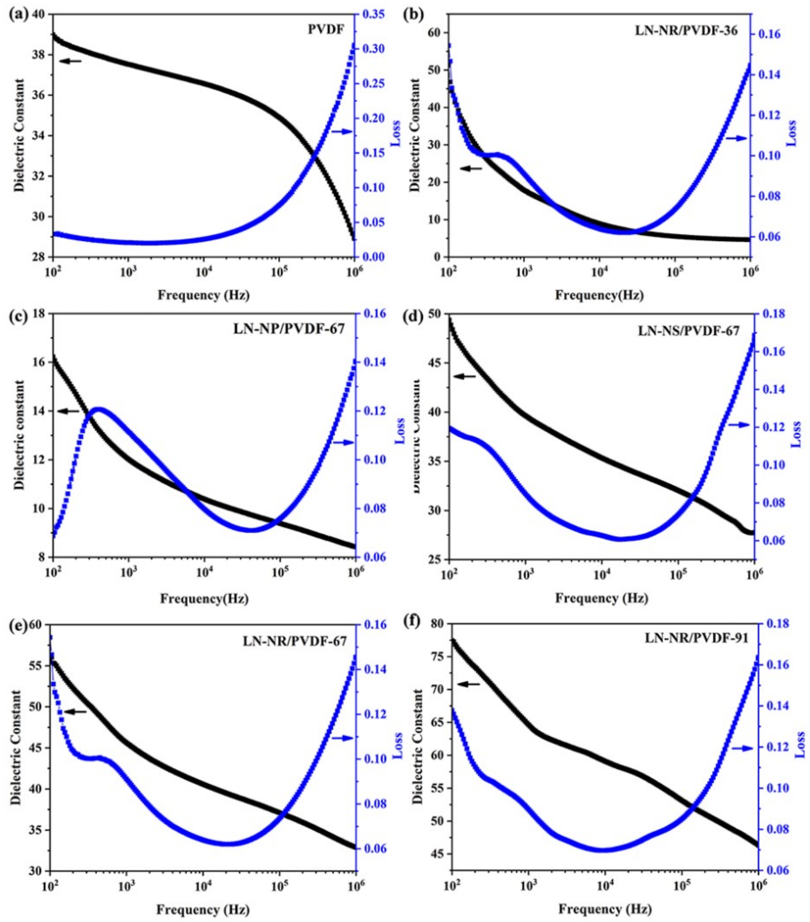


Table S2. Parameters used to calculate the flexoelectric coefficients of the pristine PVDF, LN-NS/PVDF-67, LN-NR/PVDF-36, LN-NR/PVDF-67 and LN-NR/PVDF-91 nanocomposites, including the distance *x* from the testing point of the tip displacement to the clamped end of the sample, the length (L) and width of the sample, and the vibration frequency.

Sample	x(cm)	L(cm)	b(cm)	*f*(Hz)
PVDF	1.61	1.51	1.52	4
LN-NS/PVDF-67	1.52	1.42	1.5	4
LN-NR/PVDF-36	1.64	1.57	1.5	4
LN-NR/PVDF-67	1.57	1.51	1.53	4
LN-NR/PVDF-91	1.6	1.5	1.5	4

Table S3. Equations used in the density functional theory (DFT) calculation, including the equations for the displacement, strain, strain gradient and fitting curve of the polarization of $LiNbO_3$ nanorods and the calculated flexoelectric coefficients and piezoelectric coefficients.

Displacement (Å) $u_z(x) = A * \cos(0.3x)$	Strain $S_5 = -0.3A * \sin(0.3x)$	Strain gradient ($Å^{-1}$) $\frac{\partial S_5}{\partial x} = -0.09A * \cos(0.3x)$	Fitting curve of P (C/m²) $P = eS_5 + \mu \frac{\partial S_5}{\partial x}$	coefficients
$u_z(x,z) = 0.5 * \cos(0.3x)$	$S_5 = -0.15 * \sin(0.3x)$	$\frac{\partial S_5}{\partial x} = -0.045 \cos(0.3x)$	$P_x = -0.003\cos(0.3x)$	$\mu_{511} = 0.06$ nC/m
			$P_y = -0.005 \sin(0.3x) - 0.004\cos(0.3x)$	$e_{25} = 0.03$ C/m² $\mu_{512} = 0.089$ nC/m
			$P_z = -0.0057 \sin(0.3x)$	$e_{35} = 0.038$ C/m²