New hybrid: [H−β−(4−Pyridyl)−Ala−OH] tetrafluoroborate - crystal structure and strong piezoelectricity

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Supplementary Information

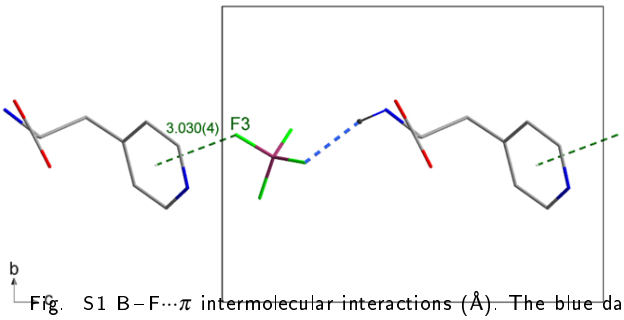

Fig. S1 B−F···π intermolecular interactions (Å). The blue dashed line indicate N−H···F hydrogen bond.

Table S1 Geometric parameters (Å, °) for $[4PyAla][BF_4]$.

O2–C1	1.248 (4)	C2–H2	1
O1–C1	1.255 (4)	C2–C3	1.548 (5)
F1–B1	1.385 (6)	N11–H11	0.88
F2–B1	1.375 (6)	N11–C16	1.355 (6)
N1–H1A	0.91	N11–C12	1.340 (6)
N1–H1B	0.91	C3–H3A	0.99
N1–H1C	0.91	C3–H3B	0.99
N1–C2	1.491 (4)	C13–H13	0.95
F3–B1	1.394 (6)	C13–C12	1.371 (6)
F4–B1	1.372 (6)	C15–H15	0.95
C1–C2	1.534 (5)	C15–C16	1.364 (6)
C14–C3	1.503 (5)	C16–H16	0.95
C14–C13	1.396 (5)	C12–H12	0.95
C14–C15	1.387 (5)		
H1A–N1–H1B	109.5	C14–C3–H3B	109.5
H1A–N1–H1C	109.5	C2–C3–H3A	109.5
H1B–N1–H1C	109.5	C2–C3–H3B	109.5
C2–N1–H1A	109.5	H3A–C3–H3B	108.1
C2–N1–H1B	109.5	C14–C13–H13	119.9
C2–N1–H1C	109.5	C12–C13–C14	120.3 (4)
O2–C1–O1	125.9 (3)	C12–C13–H13	119.9
O2–C1–C2	117.3 (3)	C14–C15–H15	119.8
O1–C1–C2	116.7 (3)	C16–C15–C14	120.5 (4)
C13–C14–C3	120.7 (3)	C16–C15–H15	119.8
C15–C14–C3	121.6 (3)	N11–C16–C15	120.4 (4)
C15–C14–C13	117.6 (4)	N11–C16–H16	119.8
N1–C2–C1	109.7 (3)	C15–C16–H16	119.8
N1–C2–H2	109.7	N11–C12–C13	120.4 (4)
N1–C2–C3	107.6 (3)	N11–C12–H12	119.8
C1–C2–H2	109.7	C13–C12–H12	119.8
C1–C2–C3	110.5 (3)	F1–B1–F3	109.5 (4)
C3–C2–H2	109.7	F2–B1–F1	110.3 (4)
C16–N11–H11	119.6	F2–B1–F3	108.0 (4)
C12–N11–H11	119.6	F4–B1–F1	109.1 (4)
C12–N11–C16	120.8 (4)	F4–B1–F2	113.0 (5)
C14–C3–C2	110.8 (3)	F4–B1–F3	106.8 (4)
C14–C3–H3A	109.5		
O2–C1–C2–N1	156.6 (3)	C3–C14–C13–C12	175.5 (4)
O2–C1–C2–C3	-84.9 (4)	C3–C14–C15–C16	-175.4 (4)
O1–C1–C2–N1	-26.5 (4)	C13–C14–C3–C2	-106.6 (4)
O1–C1–C2–C3	92.0 (4)	C13–C14–C15–C16	1.4 (5)
N1–C2–C3–C14	177.4 (3)	C15–C14–C3–C2	70.1 (4)
C1–C2–C3–C14	57.7 (4)	C15–C14–C13–C12	-1.3 (5)
C14–C13–C12–N11	-0.1 (6)	C16–N11–C12–C13	1.4 (6)
C14–C15–C16–N11	-0.1 (6)	C12–N11–C16–C15	-1.3 (6)

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Table S2 Geometric details of the B–F···π intermolecular interactions (Å, °).

	Y–X···Cg	X···Cg	Y···Cg	γ	Y–X···Cg	Y–X, π
$[4PyAla][BF_4]$	B1–F3···Cg^{ix}	3.030(4)	4.117(6)	8.04	133.6(3)	39.44

Symmetry code: (ix) x, y, -1+z. Cg is the centroid of the pyridine ring;
γ - angle between Cg···X vector and ring normal;
Y–X, π - angle of the Y···X bond
with the π - plane (i.e. Perpendicular = 0°, Parallel =0°). height

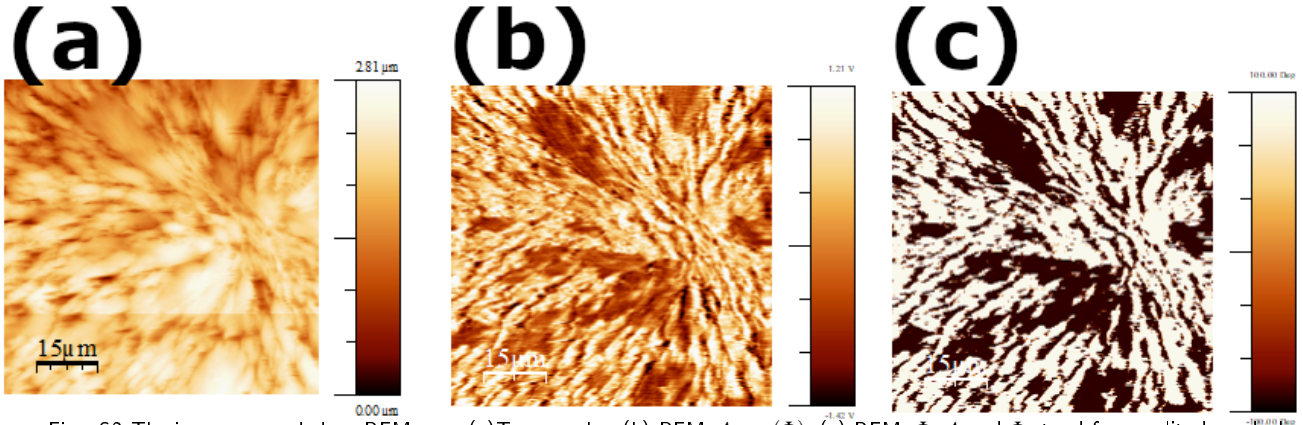

Fig. S2 The images recorded on PFM scan (a)Topography; (b) PFM, $A \cdot \cos(\Phi)$; (c) PFM, Φ. A and Φ stand for amplitude and phase, respectively

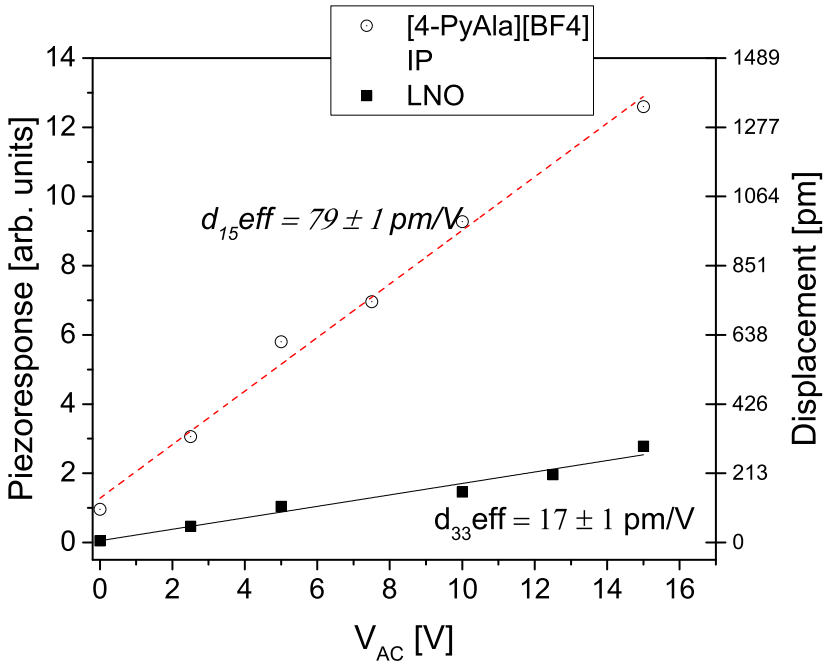

Fig. S3 Driving voltage dependence of in-plane piezoresponse of LNO and $[4PyAla][BF_4]$.