Supporting Information

High temperature molecular-based phase transition compounds with tunable and switchable dielectric properties

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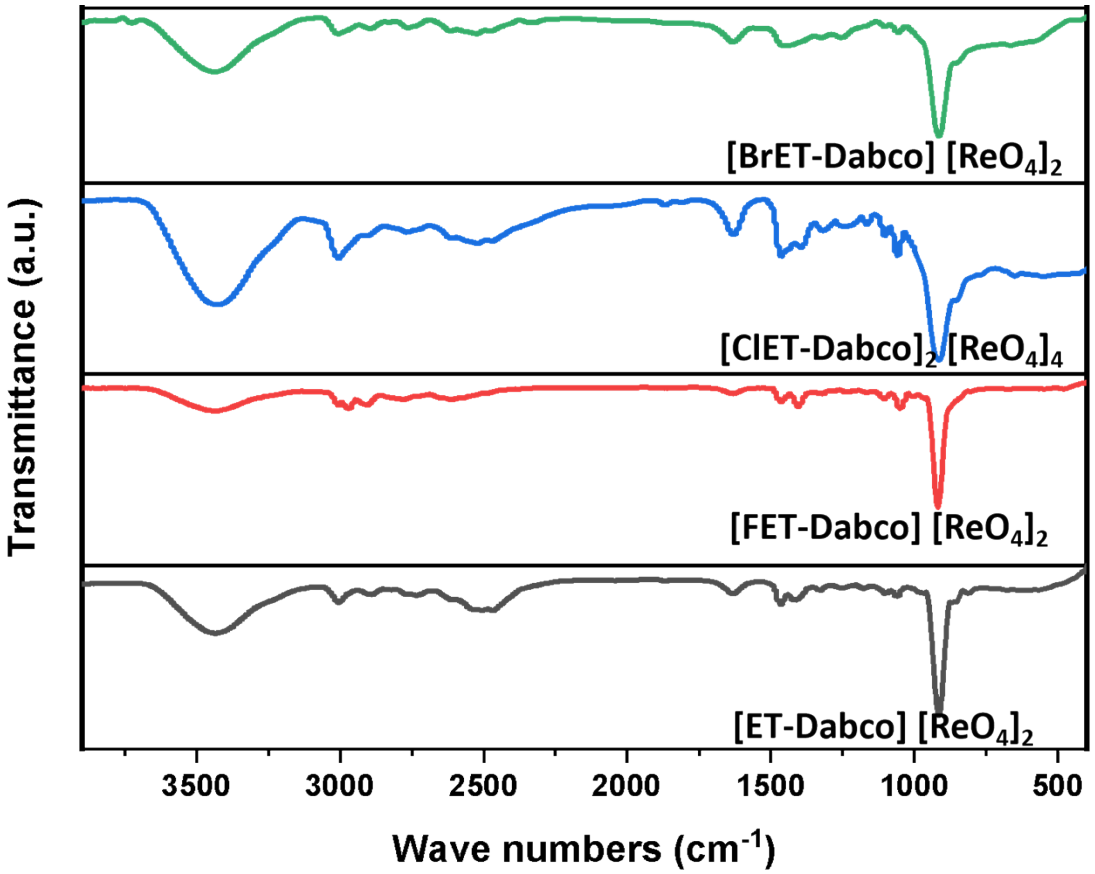

Fig. S1 Infrared (IR) spectra of [Et-Dabco] $[ReO_4]_2$, [FEt-Dabco] $[ReO_4]_2$, [ClEt-Dabco] $[ReO_4]_2$ and [BrEt-Dabco] $[ReO_4]_2$. in KBr pellet recorded on a Shimadzu model IR-60 spectrometer at 293 K.

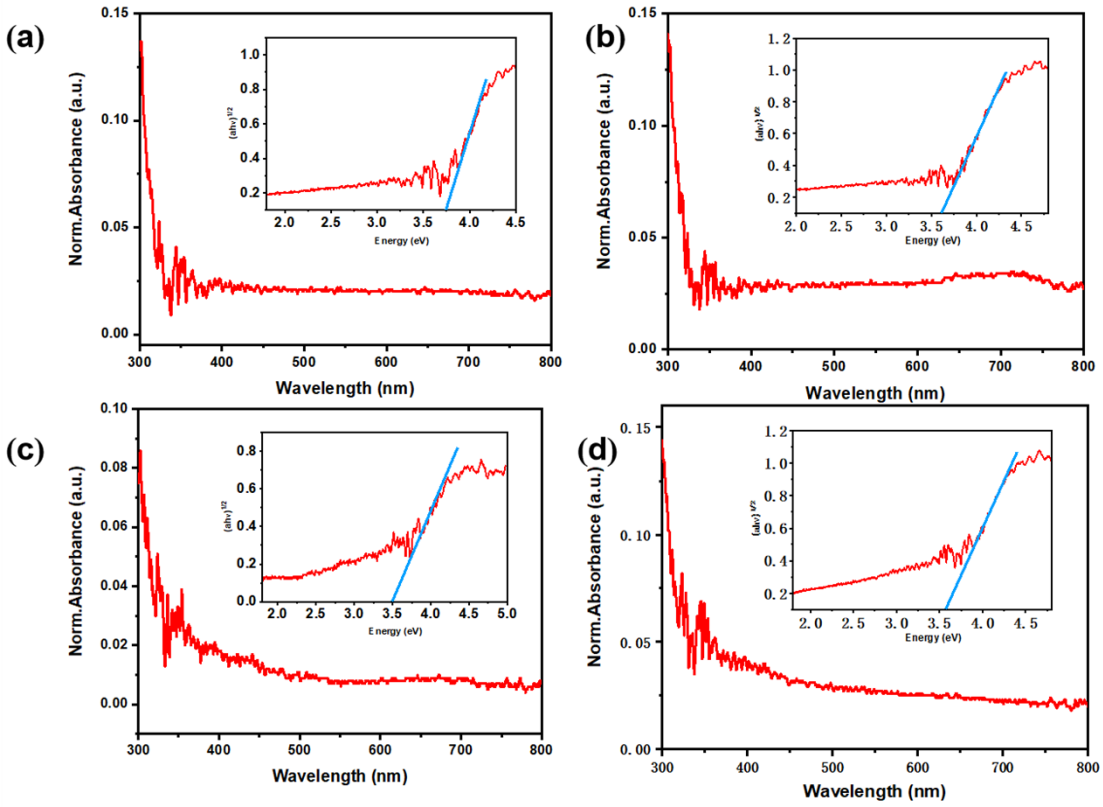

Fig. S2 UV−vis absorbance spectra of (a) [Et-Dabco] $[ReO_4]_2$, (b) [FEt-Dabco] $[ReO_4]_2$, (c) [ClEt-Dabco] $[ReO_4]_2$ and (d) [BrEt-Dabco] $[ReO_4]_2$. The inset shows the Tauc plot for determining the band gap with 3.75 eV, 3.61 eV, 3.52 eV and 3.57 eV.

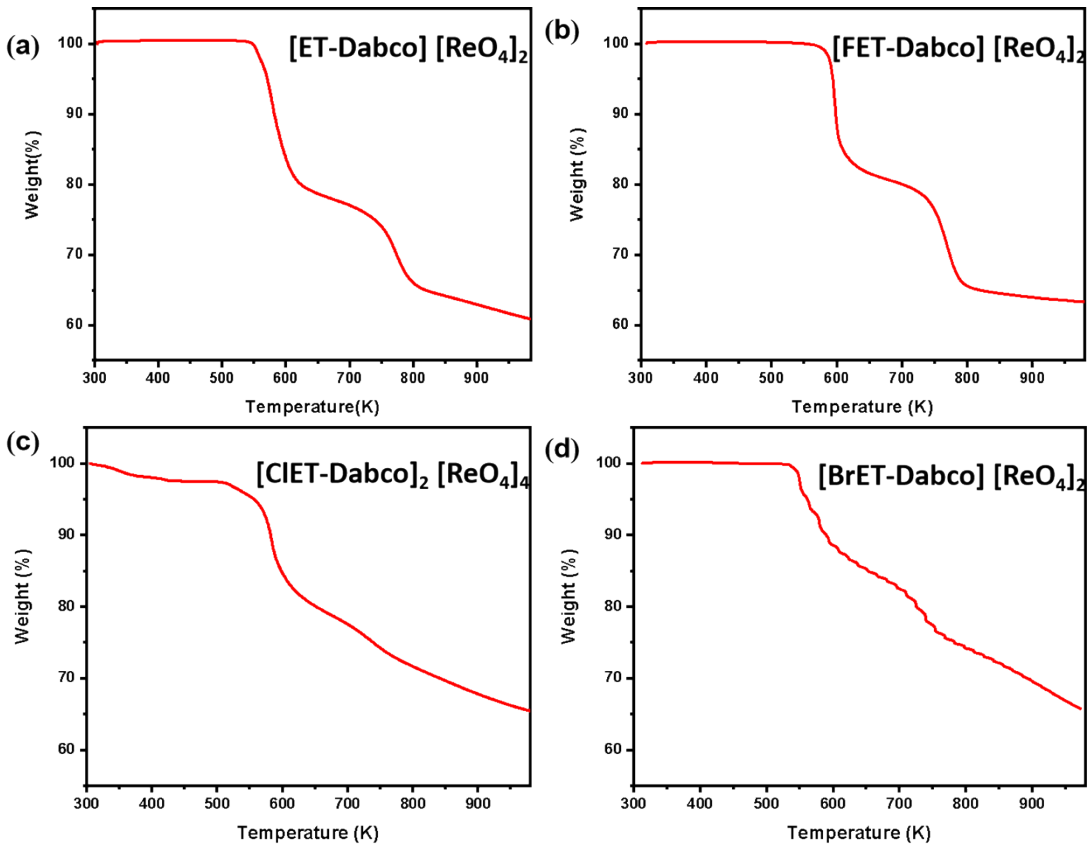

Fig. S3 The TG curves for(a) [Et-Dabco] $[ReO_4]_2$, (b) [FEt-Dabco] $[ReO_4]_2$, (c) [ClEt-Dabco] $[ReO_4]_2$ and (d) [BrEt-Dabco] $[ReO_4]_2$, indicating the decent thermal stability of the four compounds.

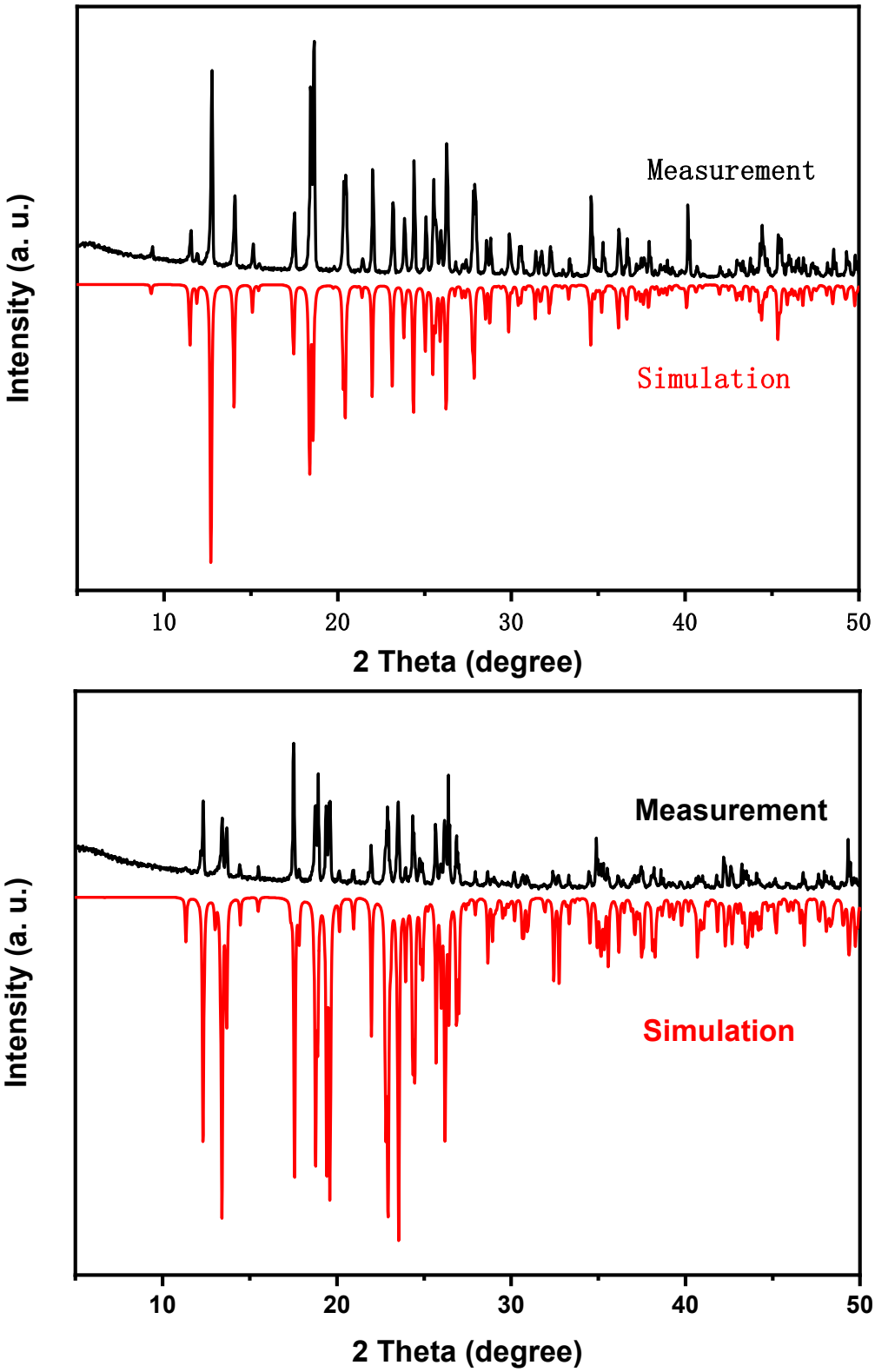

Fig. S4 Experimental powder X-ray diffraction patterns of [ClEt-Dabco] $[ReO_4]_2$ and [BrEt-Dabco] $[ReO_4]_2$ match very well with the simulated ones based on the crystal structures at 296 K.

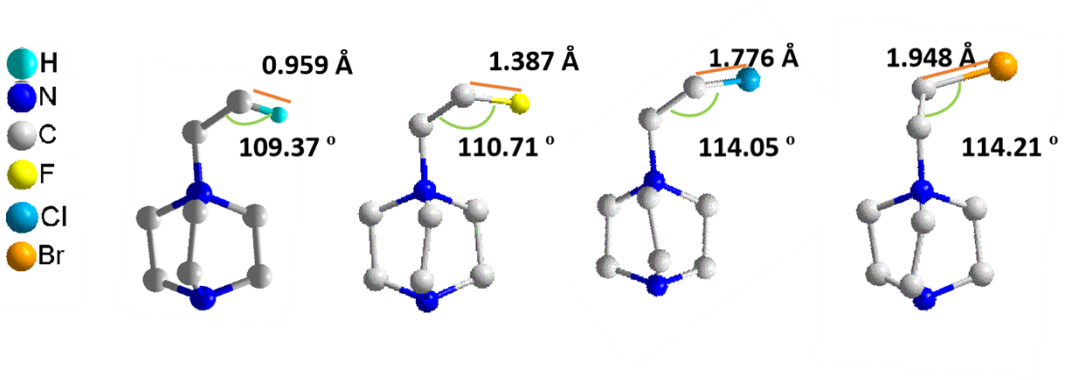

Fig. S5 Comparison of the bond angles and bond length of[Et-Dabco] $[ReO_4]_2$, [FEt-Dabco] $[ReO_4]_2$, [ClEt-Dabco] $[ReO_4]_2$ and [BrEt-Dabco] $[ReO_4]_2$ at the 296 K. All hydrogen atoms were omitted for clarity.

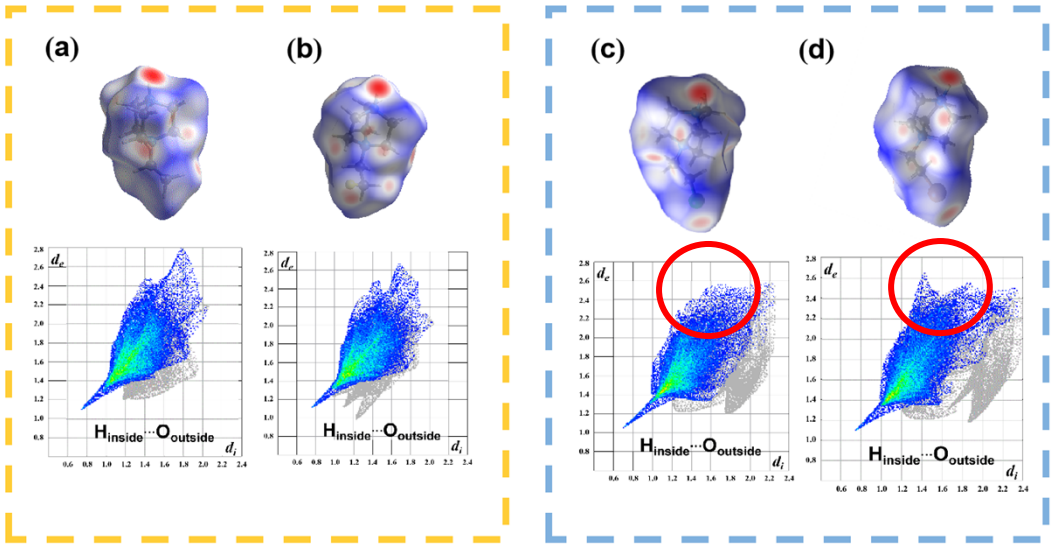

Fig. S6 At 296 K, the close contacts between $H_{inside}\cdots O_{outside}$ of [Et-Dabco] $[ReO_4]_2$ (a), [FEt-Dabco] $[ReO_4]_2$ (b), [ClEt-Dabco] $[ReO_4]_2$ (c) and [BrEt-Dabco] $[ReO_4]_2$ (d), respectively. The intensity of molecular interaction is mapped onto the Hirshfeld surface by using a red-blue-white color scheme: where the white regions exactly correspond to the distance of Van der Waals contact, the blue regions correspond to longer contacts, and the red regions represent closer contacts. In 2D fingerprint plots, each point represents an individual pair (d_i, d_e), reflecting the distances to the nearest atom inside (d_i) and outside (d_e) of the Hirshfeld surface, and the frequency of occurrence for these points corresponds to the colors from blue (low), through green, to red (highest).

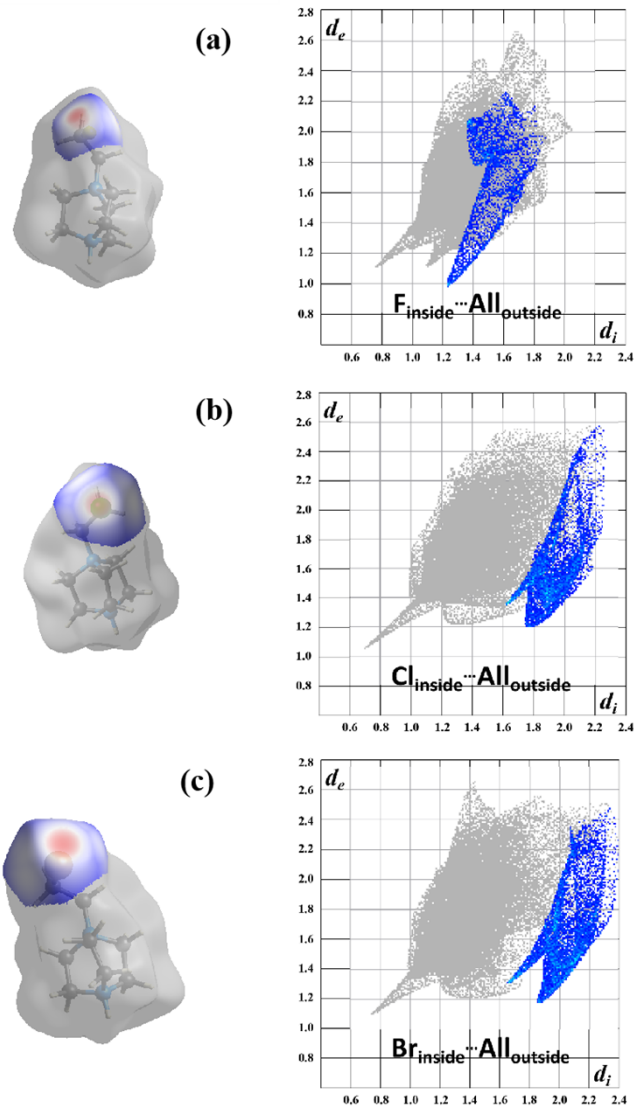

Fig. S7 Highlight close contact from elements of F_{inside}– $All_{outside}$, Cl_{inside}–$All_{outside}$ and Br_{inside}–$All_{outside}$ for (a) [FEt-Dabco] $[ReO_4]_2$, (b) [ClEt-Dabco] $[ReO_4]_2$ and (c) [BrEt-Dabco] $[ReO_4]_2$.

Formula	$C_8H_{18}N_2O_8Re_2$	$C_8H_{17}FN_2O_8Re_2$	$C_8H_{17}ClN_2O_8Re_2$	$C_8H_{17}BrN_2O_8Re_2$
Formula weight	642.64	659.63	667.09	721.55
Temperature	296K	296K	296K	296K
Crystal system	orthorhombic	orthorhombic	triclinic	triclinic
Space group	Pbca	Pbca	P-1	P-1
a/Å	10.2360(13)	10.1928(5)	8.8362(5)	7.6333(13)
b/Å	14.7742(19)	14.8794(6)	12.7362(5)	8.2742(14)
c/Å	19.084(2)	19.0803(8)	13.7512(5)	13.236(2)
α/deg	90	90	91.289(2)	90.191(2)
β/deg	90	90	94.366(2)	93.865(2)
γ/deg	90	90	96.252(2)	109.561(2)
Volume/$Å^3$	2886.1(6)	2893.8(2)	1533.15(12)	785.7(2)
Z	8	8	4	2
Densityg/cm^3	2.958	3.028	2.933	3.05
R1[I>=2σ (I)]	0.0358	0.0159	0.0428	0.024
wR2[I>=2σ (I)]	0.0819	0.0327	0.0695	0.0593
GOF	1.065	1.075	1.133	1.075

Table S1 Crystal data and structure refinements for compounds **1-4**