Supporting Information

Thermally stable Indium based metal–organic frameworks with high dielectric permittivity

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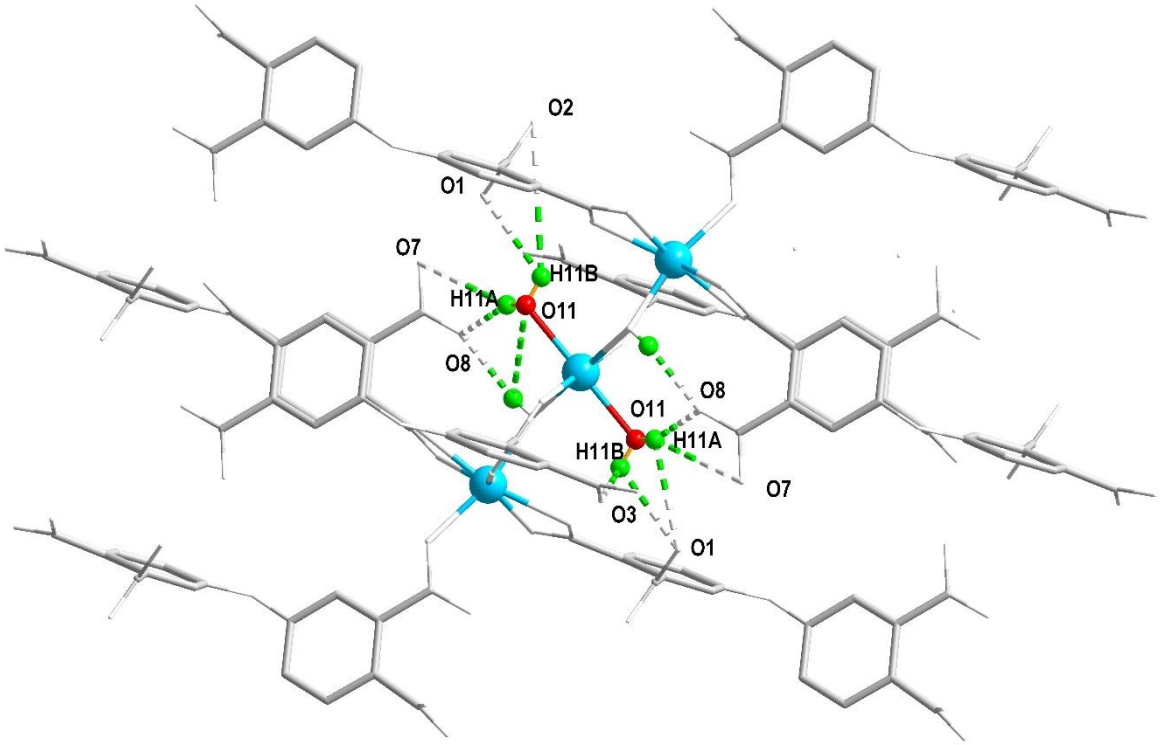

Fig. S1 Hydrogen bonding interactions of comound **1** (O8−H11A•••O11 = 1.89 Å; O2−H11B•••O11 = 3.90 Å; O8−H11B•••O11 = 2.69 Å; O8−H10A•••O10 = 2.10 Å; O11−H10A•••O10 = 2.90 Å; O7−H11A•••O11 = 3.20 Å; O7−H11•••BO11 = 3.05 Å; O1−H11A•••O11 = 2.83 Å; O1−H11B•••O11 = 2.66 Å.

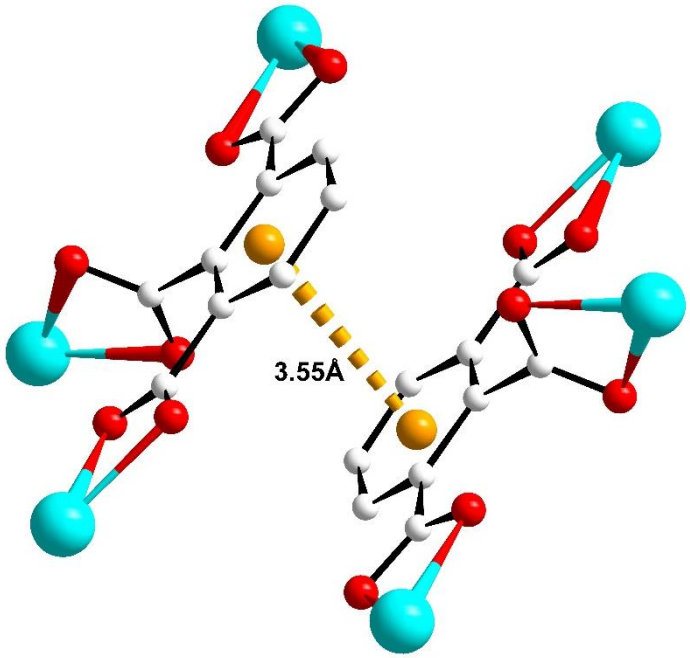

Fig. S2 The weak parallel-displaced π···π stacking interactions in between the neighboring btc ligands in compound **2**.

Dielectric relaxation

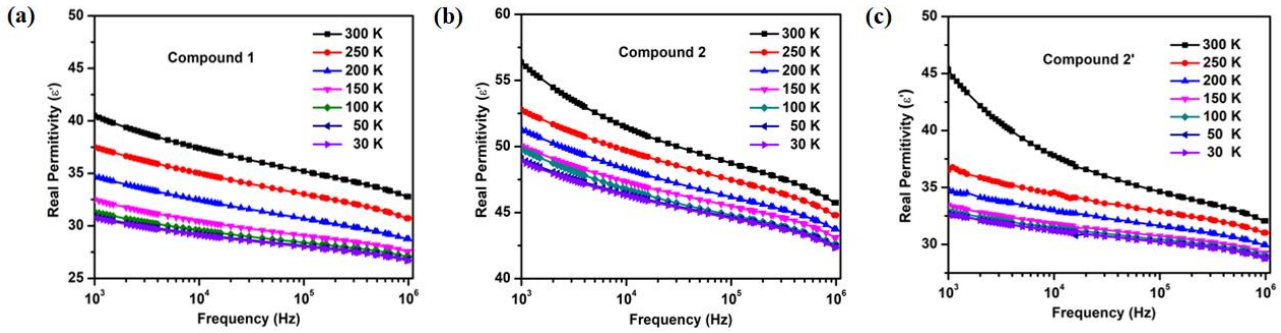

Fig. S3 Frequency dependent permittivity (ε′) of compound **1** (a), compound **2** (b), and compound **2'** (c) at different temperatures.

Dielectric loss versus frequency

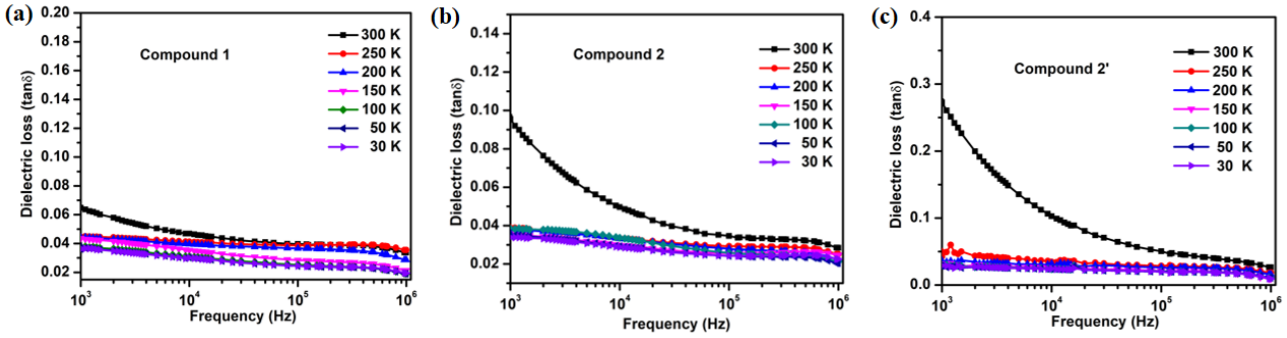

Fig. S4 Frequency dependent dielectric loss (tanδ) of compound **1** (a), compound **2** (b), and compound **2'** (c) at different temperatures.

Electrical conductivity versus temperature

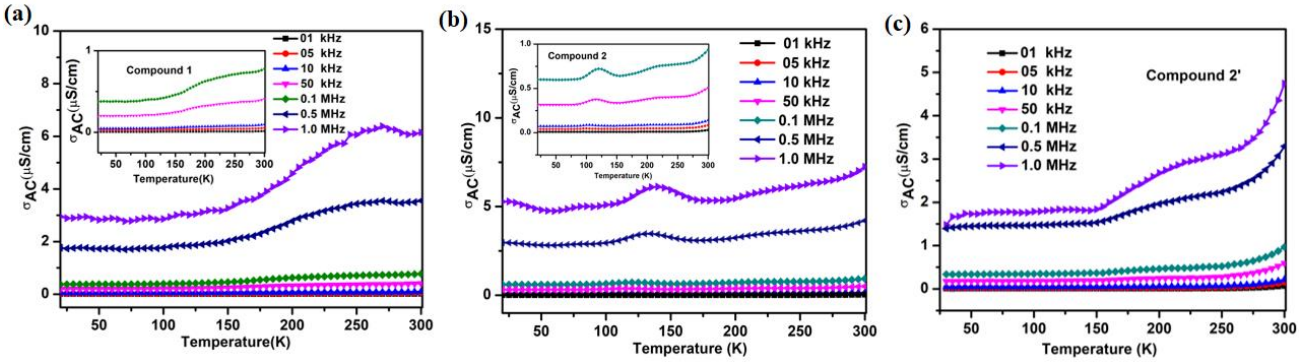

Fig. S5 temperature dependent electrical conductivities of compound **1** (a), compound **2** (b), and compound **2'** (c) at different frequencies.

Electrical conductivity versus frequency

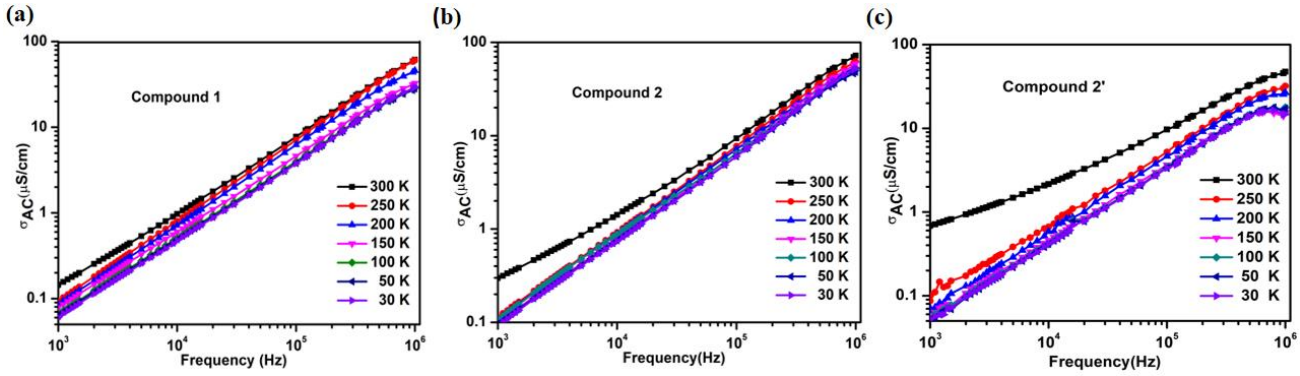

Fig. S6 Frequency dependent electrical conductivities of compound **1** (a), compound **2** (b), and compound **2'** (c) at different temperatures.

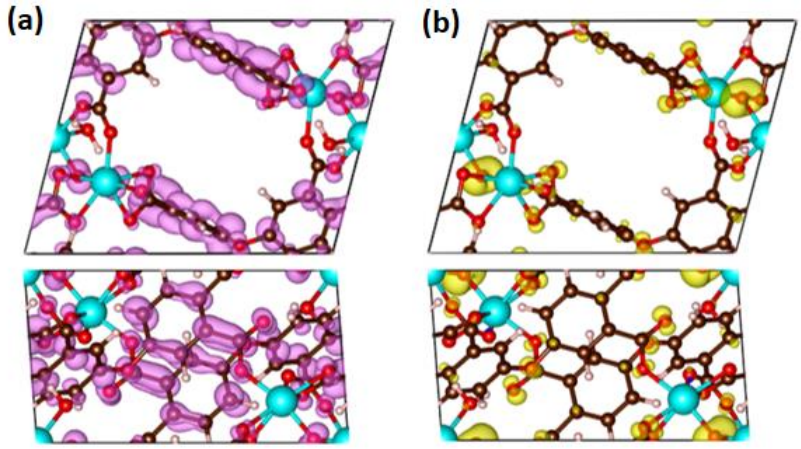

Fig. S7 The side (top panel) and top (bottom panel) views of orbital feature for the (a) CBM and (b) VBM of compound **1**

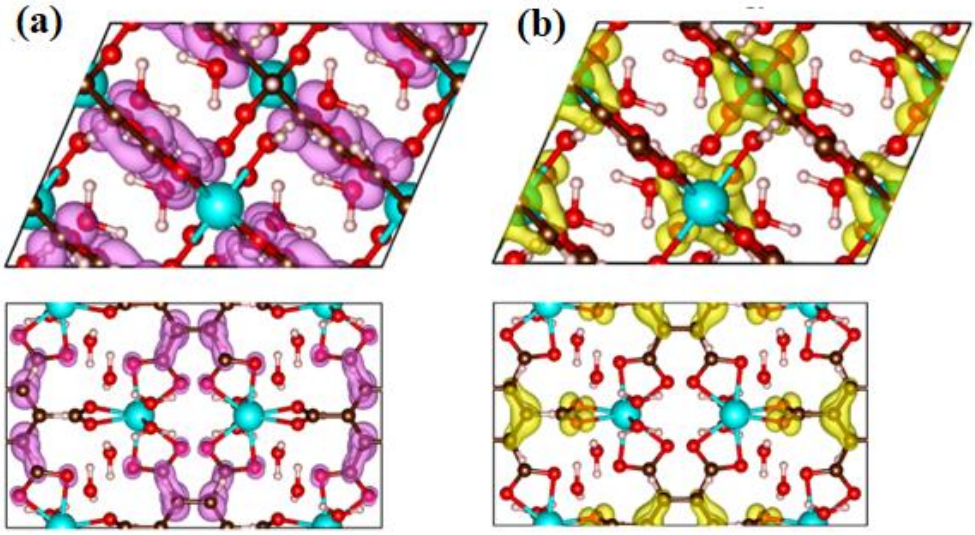

Fig. S8 The side (top panel) and top (bottom panel) views of orbital feature for the (a) CBM and (b) VBM of compound **2**

Crystal Data of Compound 1 (CCDC 1996451)

Table 1. Crystal data and structure refinement for compound **1**

Empirical formula	C32 H26 In3 Na O26
Formula weight	1193.98
Temperature	200(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	$P\bar{1}$
Unit cell dimensions	a = 7.4109(4) Å
	b = 10.7283(8) Å
	c = 13.1626(7) Å
	β = 90.383(2)°
Volume	981.17(10) Å^3
Z	1
Density (calculated)	2.021 Mg/m^3
Absorption coefficient	1.859 mm^{-1}
F(000)	584
Crystal size	0.22 x 0.03 x 0.02 mm^3
Theta range for data collection	2.84 to 25.05°
Index ranges	-8<=h<=8, -12<=k<=12, -15<=l<=15
Reflections collected	18965
Independent reflections	3446 [R(int) = 0.0569]
Completeness to theta = 25.05°	99.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7452 and 0.5995
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3455 / 7 / 288
Goodness-of-fit on F^2	1.049
Final R indices [$I > 2\sigma(I)$]	R1 = 0.0331, wR2 = 0.0793
R indices (all data)	R1 = 0.0409, wR2 = 0.0846
Largest diff. peak and hole	1.502 and -0.861 e.Å^{-3}

[a] $R_1 = \Sigma||F_0| - |F_c||/\Sigma|F_0|$; $wR_2 = [\Sigma w(F_0^2 - Fc^2)_2/\Sigma w(F_0^2)_2]^{1/2}$

Crystal Data of Compound 2 (CCDC 1996452)

Table 2. Crystal data and structure refinement for compound **2**

Empirical formula	C9 H11 In O10
Formula weight	394.00
Temperature	200(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	*C*2/*c*
Unit cell dimensions	a = 10.3577(5) Å
	b = 15.9403(8) Å
	c = 7.2865(3) Å
	β = 113.346(1)°
Volume	1104.54(9) $Å^3$
Z	4
Density (calculated)	2.369 Mg/m^3
Absorption coefficient	2.197 mm^{-1}
F(000)	776
Crystal size	0.25 x 0.21 x 0.11 mm^3
Theta range for data collection	2.49 to 25.05°
Index ranges	-12<=h<=12, -18<=k<=18, -8<=l<=8
Reflections collected	9865
Independent reflections	969 [R(int) = 0.0332]
Completeness to theta = 25.05°	98.3%
Absorption correction	multi-scan
Max. and min. transmission	0.7942 and 0.6097
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	969 / 0 / 93
Goodness-of-fit on F^2	1.029
Final R indices [$I > 2\sigma(I)$]	R1 = 0.0113, wR2 = 0.0284
R indices (all data)	R1 = 0.0115, wR2 = 0.0285
Largest diff. peak and hole	0.275 and –0.345 e.$Å^{-3}$

[a] $R_1 = \Sigma||F_0| - |F_c||/\Sigma|F_0|$; $wR_2 = [\Sigma w(F_0^2 - Fc^2)_2/\Sigma w(F_0^2)_2]^{1/2}$