Electronic Supplementary Information:

New Potential Nonlinear Optical Hybrid Semi-Organic Crystal of $ZnMnCl_2(TPPO)_4$ with attractive physical properties

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The Captions for ESI

Fig. S1 The simulated appearance of crystal and the determined facets.

Fig. S2 The photograph of the growing $MnZnCl_4(TPPO)_4$ crystal.

Fig. S3 The UV-vis Spectrum of $ZnCl_2(TPPO)_2$.

Table S1 Crystal data and structure refinements for $ZnCl_2(TPPO)_2$

Table S2 XRF- SQX calculation of $MnZnCl_4(TPPO)_4$.

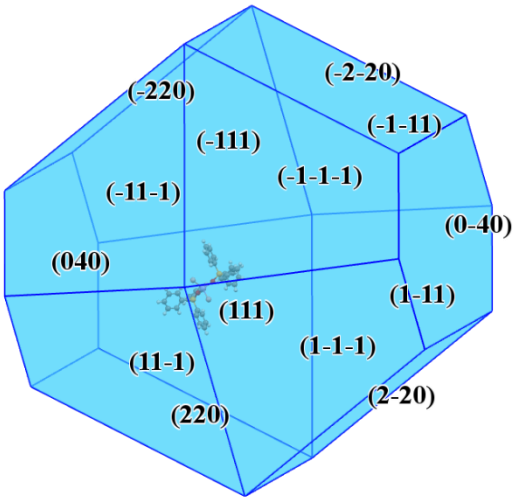

Fig. S1 The simulated appearance of crystal and the determined facets

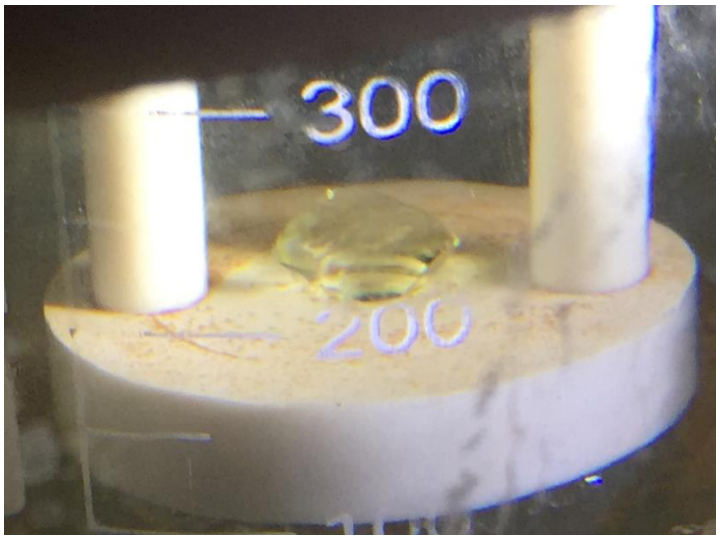

Fig. S2 The photograph of the growing $ZnMnCl_4(TPPO)_4$ crystal.

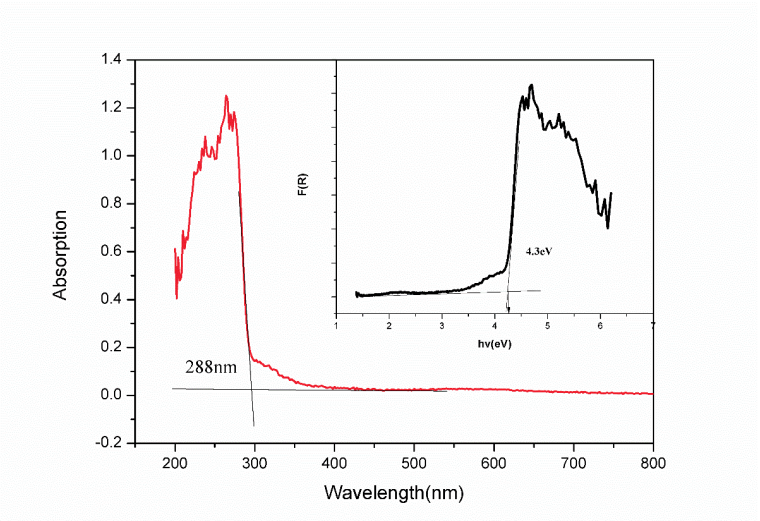

Fig. S3 The UV-vis Spectrum of $ZnCl_2(TPPO)_2$ powder.

Table S1 Crystal data and structure refinements for $ZnCl_2$ $(TPPO)_2$

Empirical formula	$ZnCl_2C_{36}H_{30}P_2O_2$
Formula weight/g·mol^{-1}	692.83
Cell setting	Orthorhombic
Space group	*F*dd2
a/Å	20.718(5)
b/Å	33.018(5)
c/Å	9.751(5)
α/°	90
β/°	90
γ/°	90
Volume / Å^3	6670(4)
Z	8
Measurement temperature	293(2)
Crystal color	colorless
Crystal size (mm^3)	0.03×0.03×0.04
Absolute structure parameter	0.015(7)
F (000)	2848
Radiation wavelength /Å	0.71073
Dcalcd (g·cm^{-3})	1.380
Limiting indices	-26<=h<=26, -42<=k<=42, -12<=l<=12
Reflections collected / unique	18771 / 3797 [R(int) = 0.0198]
μ (mm^{-1})	1.024
θ range (°)	2.32 ~27.55
Data / restraints / parameters	3797 / 1 / 196
Gof	1.052
R1, wR2 [I >2σ(I)]	R1 = 0.0203, wR2 = 0.0555
R1, wR2 (all data)	R1 = 0.0214, wR2 = 0.0559
Extinction coefficient	0.00021(5)
Min/Max Δρ/eÅ^{-3}	-0.191/ 0.230

[a]$w = 1/[s^2(Fo^2)+(0.0361P)^2+0.000P]$, where $P = (Fo^2+2Fc^2)/3$.

Table S2 XRF- SQX calculation of $MnZnCl_4(TPPO)_4$

Component	Result (mass %)	Limit of detection	Elements line	Intensity	w/o
C	51.1	0.20519	C-KA	2.3106	30.3435
P	25.2	0.01973	P-KA	89.9980	14.9580
Mn	9.94	0.00712	Mn-KA	32.5832	5.9055
Zn	13.8	0.00533	Zn-KA	115.0305	8.2268