Electronic Supporting Information

AIn$_3$Si$_4$P$_9$ (A = Ca, Sr): Quaternary Phosphides with Double-Helix Structures Exhibiting High Laser-Induced Damage Thresholds

Ming-Shu Zhang,[a,b] Bin-Wen Liu,[a] * Xiao-Ming Jiang,[a] and Guo-Cong Guo[a] *

[a] State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian 350002, P. R. China

[b] University of Chinese Academy of Sciences, Beijing 100190, P. R. China

* Guo-Cong Guo: gcguo@fjirsm.ac.cn; Bin-Wen Liu: bwliu@fjirsm.ac.cn.

Table of Contents

1. Figures and Tables.

Atomic %	Ca	In	Si	P
EDS (ave.)	1.0	2.9	5.0	9.7

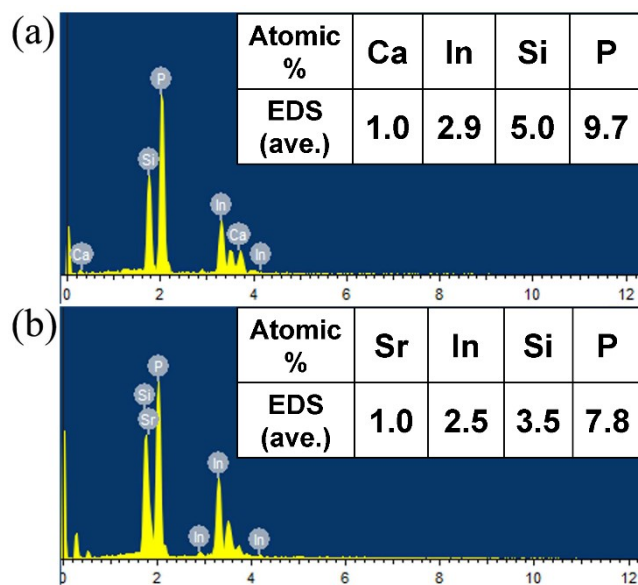| Atomic %	Sr	In	Si	P
EDS (ave.)	1.0	2.5	3.5	7.8

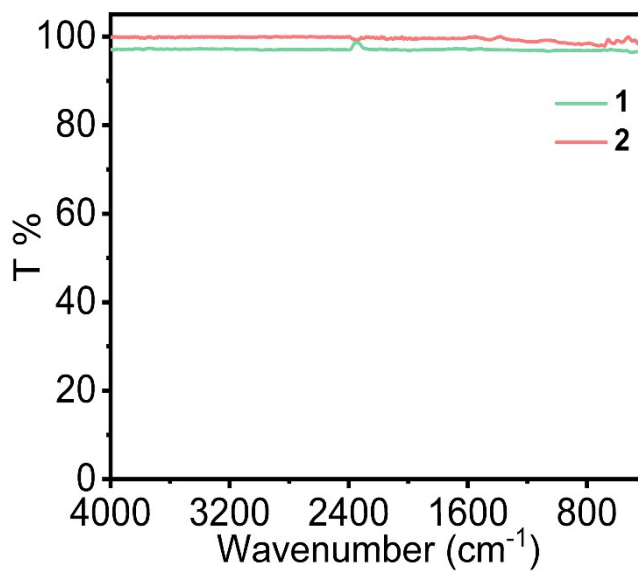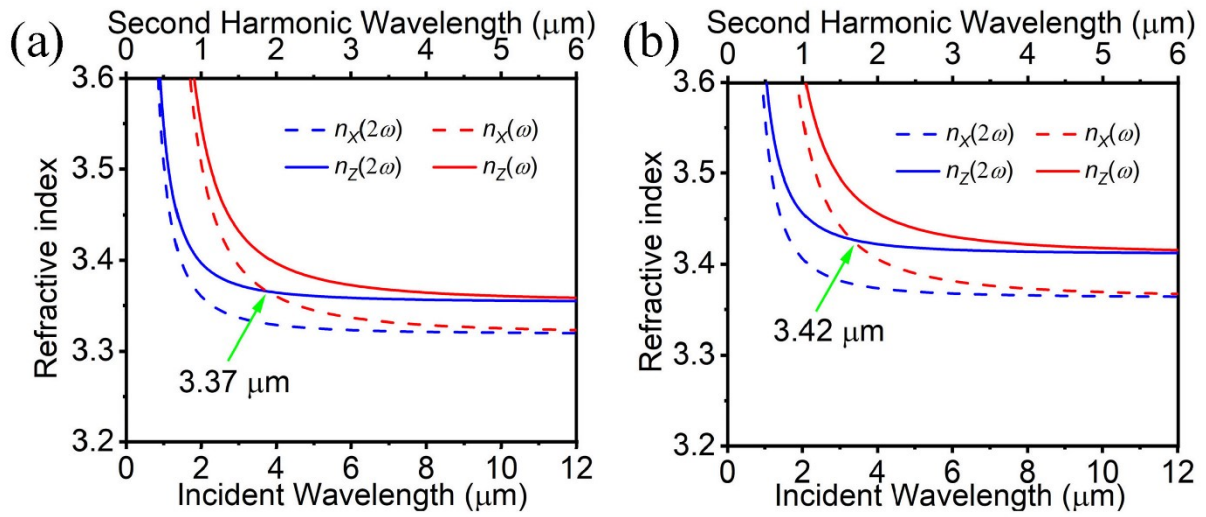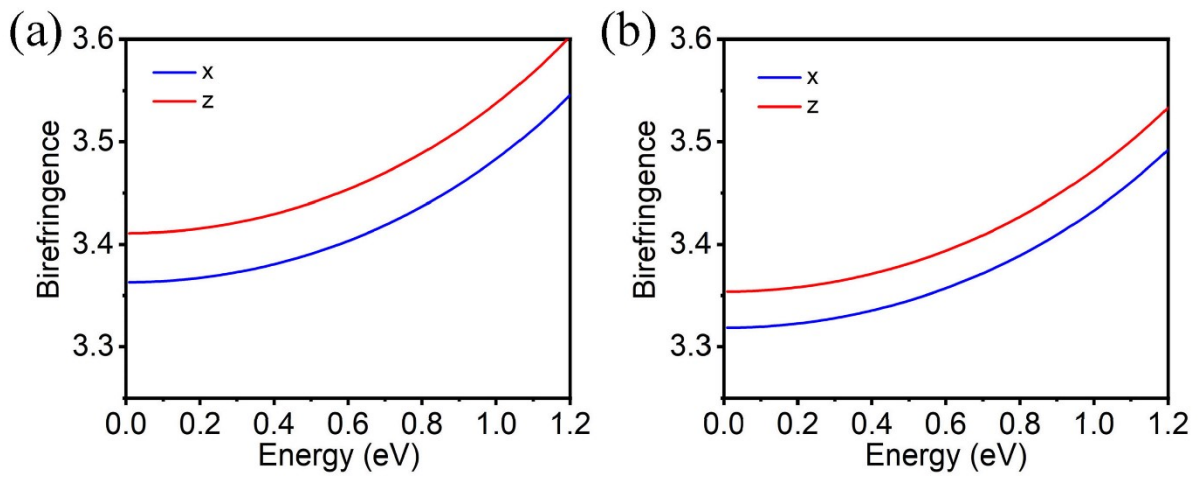**Fig. S1** EDS of single crystal of **1** (a) and **2** (b).

Fig. S2 IR spectra of **1** and **2**.

Fig. S3 Frequency-dependent refractive indexes of **1** (a) and **2** (b) along symmetry-independent *a* and *c* axes.

Fig. S4 Calculated birefringence of **1** (a) and **2** (b).

Table S1 Crystal data and structure refinement results for **1** and **2**.

Empirical formula	$CaIn_3Si_4P_9$ (**1**)	$SrIn_3Si_4P_9$ (**2**)
CCDC	2124618	2124617
Fw	775.63	823.17
Temperature (K)	293(2)	293(2)
Space group	$P4_12_12$	$P4_12_12$
a (Å)	12.2959(3)	12.4702(3)
b (Å)	12.2959(3)	12.4702(3)
c (Å)	9.7043(4)	9.6358(4)
Volume (Å^3)	1467.18(12)	1498.42(10)
Z	1	1
D_{calcd} (g cm^{-3})	3.511	3.649
μ (mm^{-1})	6.301	9.348
GOF on F^2	1.002	1.049
$R_1{}^a$ ($I > 2\sigma$ (I))	0.0477	0.0326
$wR_2{}^b$ ($I > 2\sigma$ (I))	0.1723	0.0826
$R_1{}^a$ (all data)	0.0542	0.0347
$wR_2{}^b$ (all data)	0.1921	0.0840
Flack	0.06(3)	0.00(3)
$\Delta\rho_{max}/\Delta\rho_{min}$ (e Å^{-3})	3.77/-3.65	1.29/-2.13

$^aR = \Sigma||F_o|-|F_c||/\Sigma|F_o|$, $^bwR = (\Sigma(w(F_o{}^2-F_c{}^2)^2)/\Sigma(w(F_o{}^2)^2))^{1/2}$.

Table S2 Fractional atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters (Å$^2 \times 10^3$) for **1** and **2**.

		1		
Atom	x	y	z	U(eq)
Ca1	5766(3)	5766(3)	0	27.4(12)
In1	3334.2(8)	327.3(9)	4734.5(11)	15.2(4)
In2	3606.3(10)	3606.3(10)	0	24.4(5)

Si1	2152(3)	1234(3)	1472(4)	9.2(8)
Si2	1006(3)	3788(3)	1590(3)	3.1(7)
P1	2584(3)	2986(3)	2075(4)	12.8(8)
P2	4639(3)	1909(3)	4672(4)	10.5(7)
P3	3812(3)	635(3)	720(3)	6.4(7)
P4	845(3)	845(3)	0	9.8(10)
P5	1583(3)	471(4)	3400(4)	20.4(9)

2

Atom	x	y	z	U(eq)
Sr1	5824.5(10)	5824.5(10)	0	22.3(4)
In1	3614.8(7)	3614.8(7)	0	18.1(3)
In2	3353.6(6)	309.6(7)	4702.4(8)	11.9(2)
Si1	2164(2)	1271(2)	1504(3)	8.1(6)
Si2	1041(2)	3818(2)	1626(3)	1.6(5)
P1	4671(2)	1829(2)	4672(3)	10.8(5)
P2	3788(2)	660(2)	718(3)	7.2(5)
P3	2583(2)	2996(2)	2114(3)	12.5(6)
P4	1617(2)	489(3)	3420(3)	15.0(6)
P5	900(2)	900(2)	0	10.3(8)

Table S3 Selected distances (Å) for **1** and **2**.

1

Bond	Distances	Bond	Distances
In1-P2	2.530(4)	Si1-P5	2.206(5)
In1-P2	2.522(4)	Si1-P3	2.290(5)
In1-P3	2.691(4)	Si1-P4	2.202(5)
In1-P5	2.519(4)	Si2-P2	2.290(5)
In2-P1×2	2.493(4)	Si2-P3	2.290(4)
In2-P5×2	2.465(5)	Si2-P1	2.227(5)
Si1-P1	2.295(5)	Si2-P3	2.288(5)

2

Bond	Distances	Bond	Distances
In1-P3×2	2.530(3)	Si1-P3	2.291(4)
In1-P4×2	2.516(3)	Si1-P4	2.191(4)
In2-P1	2.507(3)	Si2-P1	2.217(4)
In2-P1	2.520(3)	Si2-P2	2.309(4)
In2-P2	2.675(3)	Si2-P3	2.311(4)
In2-P4	2.504(3)	Si2-P3	2.230(4)
Si1-P2	2.292(4)		

Table S4 Selected angles for **1** and **2**.

1

Atom-Atom-Atom	Angle/°	Atom-Atom-Atom	Angle/°
P5-Si1-P4	103.8(16)	P4-In1-P4	109.71(14)

Atom-Atom-Atom	Angle/°	Atom-Atom-Atom	Angle/°
P5-Si1-P3	122.16(16)	P4-In1-P3	120.57(9)
P4-Si1-P3	105.77(15)	P4-In1-P3	98.84(9)
P5-Si1-P2	110.33 (13)	P4-In1-P3	98.84(9)
P4-Si1-P2	113.86(16)	P4-In1-P3	120.57(9)
P3-Si1-P2	101.27(15)	P3-In1-P3	109.77(14)
P1-Si2-P3	112.78(15)	P4-In2-P1	119.56(10)
P1-Si2-P2	110.29(14)	P4-In2-P1	114.61(9)
P3-Si2-P2	112.13(15)	P1-In2-P1	108.00(11)
P1-Si2-P2	113.50(15)	P4-In2-P2	101.39(10)
P3-Si2-P2	111.33(15)	P1-In2-P2	103.19(9)
P2-Si2-P2	95.66(14)	P1-In2-P2	108.78(9)

2

Atom-Atom-Atom	Angle/°	Atom-Atom-Atom	Angle/°
P4-Si1-P5	103.1(2)	P5-In1-P2	118.51(14)
P4-Si1-P3	111.93(17)	P5-In1-P2	113.79(12)
P5-Si1-P3	114.6(2)	P2-In1-P2	110.83(14)
P4-Si1-P1	122.56(19)	P5-In1-P3	99.81(13)
P5-Si1-P1	104.9(2)	P2-In1-P3	102.78(12)
P3-Si1-P1	100.16(19)	P2-In1-P3	109.56(11)
P1-Si2-P2	111.83(19)	P5-In2-P5	107.54(19)
P1-Si2-P3	112.75(18)	P5-In2-P1	98.84(12)
P2-Si2-P3	112.41(18)	P5-In2-P1	121.55(12)

P1-Si2-P3	109.69(19)	P5-In2-P1	121.55(12)
P2-Si2-P3	114.20(18)	P5-In2-P1	98.84(12)
P3-Si2-P3	94.92(17)	P1-In2-P1	110.12(18)