

Journal Name

ARTICLE

## Controllable Seeded Flux Growth and Optic-electric Properties of Bulk o-SiP Crystals

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### Supporting information

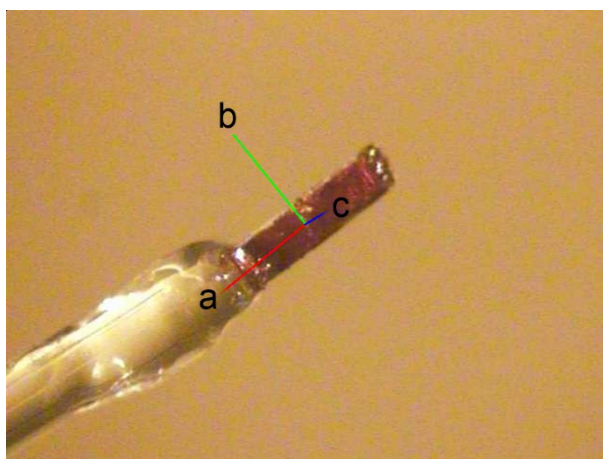


Figure S1. The crystalline orientation of single-crystal flake was determined by single-crystal X-ray.

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Electronic Supplementary Information (ESI) available: [details of any supplementary information available should be included here]. See DOI: 10.1039/x0xx00000x

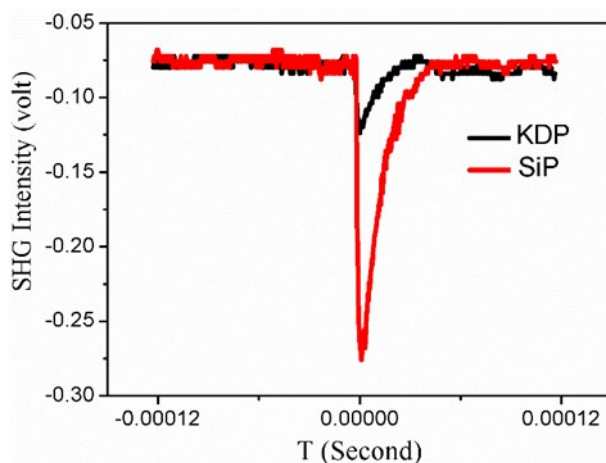


Figure S2. Oscilloscope traces of SHG signals for o-SiP with KDP as a reference.

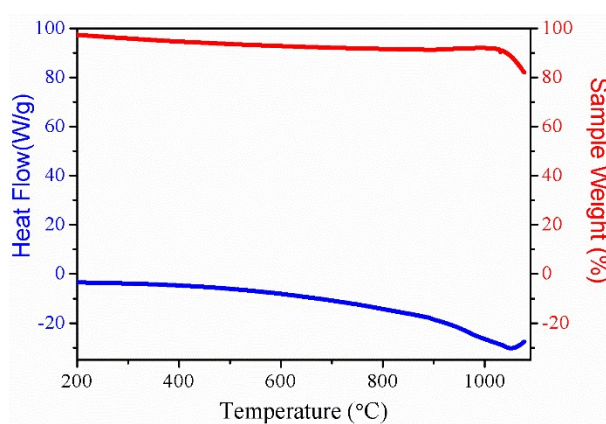


Figure S3. DSC/TG data of o-SiP. Blue curve represents DSC and red curve represents TG. The sample decomposes at 1045 °C, where the endothermic peak in the DSC curve together with the dramatic weight loss indicates decomposition of the crystal.

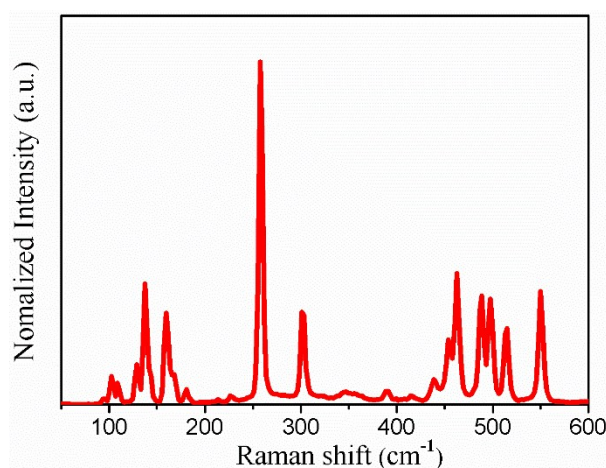


Figure S4. Raman spectrum of o-SiP crystal grown by flux method.

Table S1. Crystallographic Data and Structure Refinement for o-SiP

Empirical formula	SiP
Formula weight	59.06
Temperature	293(2) K

Wavelength (Å)	0.71073
Crystal system	Orthorhombic
Space group	Cmc2 <sub>1</sub>
Unit cell dimensions (Å)	<i>a</i> = 3.5255(6) <i>b</i> = 20.563(4) <i>c</i> = 13.666(2)
Volume (Å <sup>3</sup> )	990.7(3)
Z, Calculated density	16, 1.584 mg/m <sup>3</sup>
Absorption coefficient	1.163 mm <sup>-1</sup>
F(000)	464
Crystal size	0.18mm × 0.12mm × 0.11mm
Theta range for data collection	1.98 to 27.47 deg.
Limiting indices	-4 ≤ <i>h</i> ≤ 4, -26 ≤ <i>k</i> ≤ 26, -17 ≤ <i>l</i> ≤ 17
Reflections collected / unique	5513 / 1310
R(int)	0.0254
Completeness to theta = 27.47	99.3 %
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	1310 / 1 / 74
Goodness-of-fit on F <sup>2</sup>	1.199
Final R indices [ <i>I</i> > 2σ( <i>I</i> )] <sup>b</sup>	R1 = 0.0215, wR2 = 0.0658
R indices (all data)	R1 = 0.0217, wR2 = 0.0660
Absolute structure parameter	0.4(3)
Extinction coefficient	0.0001(4)
Largest diff. peak and minimum	0.495 and -0.443 e.Å <sup>-3</sup>

Table S2. Hall effect measurements

Test condition		Result	
I (nA)	10	Nb (cm <sup>-3</sup> )	1.214E+10
B (T)	0.55	u (cm <sup>2</sup> ·V <sup>-1</sup> ·s <sup>-1</sup> )	2.034E+03
Thickness (μm)	320.00	Rho (Ω·cm)	2.527E+05
Delay Time (s)	0.100	RH (cm <sup>3</sup> ·C <sup>-1</sup> )	5.141E+08
Measure Time (h)	0.100	RHA (cm <sup>3</sup> ·C <sup>-1</sup> )	4.116E+08
T(K)	300	RHB (cm <sup>3</sup> ·C <sup>-1</sup> )	6.166E+08