Pressure-engineered optical properties and emergent superconductivity in chalcopyrite semiconductor ZnSiP$_2$

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Abstract
Chalcopyrite II-IV-V$_2$ semiconductors are promising materials in nonlinear optical, optoelectronic, and photovoltaic applications. In this work, pressure-tailored optical properties as well as pressure-driven emergent superconductivity in chalcopyrite ZnSiP$_2$ are reported via photoluminescence (PL) spectroscopy and electrical transport experiments. During compression, the PL peak energy exhibits a plateau between 1.4 and 8.7 GPa, which is accompanied by a piezochromic transition and correlated with the progressive development of cation disorder. Upon further compression across a phase transition from tetragonal to cubic rock-salt structure, superconductivity with a critical temperature $T_c$ $\sim$ 8.2 K emerges immediately. $T_c$ decreases in the range of 24.6–37.1 GPa but inversely increases at higher pressures, thereby exhibiting an unusual V-shaped superconducting phase diagram. These findings present vivid structure–property relationships, which not only offer important clues to optimize the optical and electronic properties, but also provide a new way to use compression to switch between different functionalities.

Introduction
As isoelectronic analogs of III–V zincblende materials, zinc-based chalcopyrites ZnXP$_n$$_2$ (X = Si, Ge, and Sn; P$_n$ = P, As, and Sb) have recently attracted great attention because of their potential technological applications in nonlinear optics, optoelectronics, and photovoltaics$^{1-10}$. For instance, ZnGeP$_2$ can be applied to nonlinear optical devices based on its large nonlinear coefficient, birefringence, and large-area growth availability$^3$. ZnSnP$_2$ is an absorber material for solar cells, whose bandgap can be effectively engineered by tuning the cation disorder$^6$. Furthermore, a recent first-principles calculation predicted that ZnSnP$_2$ displays large shift-current conductivity, a bulk photovoltaic phenomenon correlated with the Berry connection between the valence and conduction bands$^{10}$. As for ZnSiP$_2$, it possesses a direct bandgap of $E_g$ $\sim$2.01 eV$^9$ and a typically cation-ordered tetragonal structure with intrinsic stability and defect tolerance$^2$. Apart from its inexpensive, earth-abundant, and nontoxic elemental constituents, ZnSiP$_2$ has become a promising candidate for transitional tandem solar cells owing to its small lattice mismatch and good refraction index matching with Si, little parasitic below-bandgap absorption, excellent photoresponse, and high open-circuit voltage$^{2,11-13}$. After disorder is introduced into the cation sublattice, ZnSiP$_2$ can be further used as a high-performance anode material for next-generation Li-ion batteries$^1$.

As one of the fundamental state parameters, pressure is an effective and clean way to tune the lattice constant, crystal structure, and electronic state, thus varying the fundamental physical properties of materials. Regarding the pressure engineering of photovoltaic and...
optoelectronic materials, various exotic phenomena have been revealed recently, including photoluminescence (PL) emission enhancement, prolonged carrier lifetime, bandgap optimization, and superconductivity. For the photovoltaic material ZnSiP₂, Bhadram et al. reported that it undergoes a phase transition from tetragonal to cubic rock-salt structure between 27 and 30 GPa, in agreement with the ab initio investigations. However, a systematic investigation of the electronic and optical properties of ZnSiP₂ under pressure is still lacking to date.

Here, we systematically investigate the pressure effect on the structural, optical, and electronic properties of the chalcopyrite semiconductor ZnSiP₂ through various experimental measurements, including synchrotron X-ray diffraction (XRD), Raman spectroscopy, PL spectroscopy, optical microscopy, and electrical transport measurements. We show that pressure-induced modulations in optical and electronic properties correlate well with the structural evolution. For the optical properties, the peak energy of the PL spectrum displays a plateau between 1.4 and 8.7 GPa due to the presence of disorder in the cation sublattice. Moreover, along with the structural phase transition from tetragonal to cubic phase, a V-shaped superconducting behavior is observed.

Materials and methods
Sample synthesis and characterization at ambient pressure

Single crystals of ZnSiP₂ were grown via a flux method. Room-temperature X-ray diffraction (XRD) patterns of single crystals were obtained by using a Rigaku X-ray diffractometer with Cu Kα radiation (λ = 1.5406 Å). The atomic proportions of the crystals were characterized by energy dispersive X-ray spectroscopy (EDXS). Absorption spectra were collected by using a UV/Vis/NIR spectrometer (CRAIC 20/30PV).

High-pressure PL spectra, Raman spectra, and X-ray diffraction measurements

High-pressure PL emission, Raman scattering, and angle-dispersive synchrotron XRD experiments were conducted on powdered single-crystal ZnSiP₂ to explore the structural stability at high pressures. The synthesized ZnSiP₂ single crystals were characterized via various experimental techniques under ambient conditions. Fig. 1a displays a single-crystal XRD pattern collected from a sample freshly cleaved from a bulk crystal, which shows a (101) orientation of the cleavage plane. The EDXS measurement reveals that the cleaved sample is off-stoichiometric with a real composition of Zn₀.92±0.02SiP₂.07±0.03. The absorption spectrum shown in Fig. 2a yields a bandgap of ~2.06 eV, consistent with that reported in recent literature. The PL spectrum at room-temperature (see Fig. 2b) features a broad emission band peaking at ~919 nm (equivalent to 1.36 eV), which can be ascribed to the donor–acceptor pair transitions via defects (vacancies and antisites).

Results and discussion

The synthesized ZnSiP₂ single crystals were characterized via various experimental techniques under ambient conditions. Fig. S1 displays a single-crystal XRD pattern collected from a sample freshly cleaved from a bulk crystal, which shows a (101) orientation of the cleavage plane. The EDXS measurement reveals that the cleaved sample is off-stoichiometric with a real composition of Zn₀.92±0.02SiP₂.07±0.03. The absorption spectrum shown in Fig. 2a yields a bandgap of ~2.06 eV, consistent with that reported in recent literature. The PL spectrum at room-temperature (see Fig. 2b) features a broad emission band peaking at ~919 nm (equivalent to 1.36 eV), which can be ascribed to the donor–acceptor pair transitions via defects (vacancies and antisites). In ref. Martinez et al. showed that the PL peak energy of ZnSiP₂ varies from 1.8 eV to 1.67 eV as the temperature is increased from 5 K to 100 K, illustrating a temperature effect on the PL peak position. Based on the data of ref. a value of ~1.4 eV at 300 K is obtained by extrapolation according to the approximate model for temperature-dependent PL spectra. These results consistently confirm the high quality of our samples.

High-pressure electrical transport measurements

High-pressure transport experiments were performed in a screw-pressure-type DAC made of CuBe alloy. A pair of anvil culets of 300 μm was used. A mixture of epoxy and fine cubic boron nitride (c-BN) powder was compressed firmly to insulate the electrodes from the steel gasket. A single-crystal flake with dimensions of ~120 × 40 × 10 μm³ was loaded together with NaCl fine powder and ruby powder. A four-probe configuration was utilized to measure the resistance of the flake, where the external magnetic field was perpendicular to the surface of the flake. The ruby fluorescence shift was used to calibrate the pressure at room-temperature in all experiments.
XRD patterns. Although peak broadening in the XRD pattern can be caused by nonhydrostatic compression associated with the PTM, similar broadening behavior was also observed by Bhadram et al.\cite{22} They used Ar and He as the PTMs, which provide better hydrostatic conditions than the silicone oil used in our case\cite{22}. The extracted lattice parameters $a$ and $c$ are displayed in the upper part of Fig. 1c. The unit-cell volume as a function of pressure can be fitted by the third-order Birch-Murnaghan equation of state\cite{30}; see the solid lines in the lower panel of Fig. 1c. The unit-cell volume as a function of pressure can be fitted by the third-order Birch-Murnaghan equation of state\cite{30}; see the solid lines in the lower panel of Fig. 1c. The fittings yield ambient pressure volume $V_0 = 302.0 (4)$ Å$^3$, bulk modulus $B_0 = 97.5(6)$ GPa, and first-order derivative of the bulk modulus at zero pressure $B_0'/0 = 6.3 (0)$ for the pristine tetragonal phase and $124.9(8)$ Å$^3$, $110.0 (1)$ GPa, and $3.4(5)$ for the high-pressure cubic phase. Note that the errors caused by Le Bail refinements and/or nonhydrostatic conditions are not included for the equation of state fitting. The structural phase transition yields a unit-cell volume contraction $\Delta V/V \sim 19.1\%$ at 27.6 GPa, similar to the case of a previous report\cite{22}.

Figure 1b depicts selective room-temperature Raman spectra of ZnSiP$_2$ at various pressures. At 0.2 GPa, the Raman vibrational modes centered at 102.0, 129.9, 185.3, 264.8, 334.4, 338.2, 344.6, 464.8, 494.8, and 519.7 cm$^{-1}$ can be assigned to $E$, $E_T$, $A_1$, $B_1$, $B_{2T}$, $E_L$, $B_{2T}$-$E_T$, and $B_{2L}$-$E_L$, respectively\cite{31}. The evolutions of these modes under pressure are qualitatively consistent with those reported in ref.\cite{22}, which were believed to accord with a scenario of a two-stage transition. Based on the model proposed by Bernard and Zunger\cite{32}, it was suggested that Zn and Si cations substitute each other in the first stage, leading to a partially cation-disordered sublattice in the low-pressure tetragonal phase. The second stage involves the structural transition from the tetragonal phase to the high-pressure cubic phase\cite{22}. The strain energy, set up by the atomic size mismatch between the Zn-P and Si-P bond lengths, could be the reason to control the nature of the state of order in chalcopyrite ZnSiP$_2$\cite{22,33}. Owing to the lattice instability caused by progressive development of cation disorder, the modes below 200 cm$^{-1}$ that
As shown in Fig. 2a, in contrast to the continuous blueshift of optical phonon modes, B1 and E demonstrate a crossover from blueshift to redshift ca. 8 and 15 GPa, respectively. Meanwhile, the FWHM of each mode shows corresponding changes. Along with the structural transition to the cubic phase upon further compression, these modes show an abrupt reduction in intensity above 27.8 GPa and completely disappear when the structural transition completes at 36.7 GPa. A similar pressure-induced two-stage order-disorder transition was also claimed in defect chalcopyrite CdAl2S417. In (MA)PbI3, the abrupt blueshift of the PL energy in perovskite (MA)PbBr3 was attributed to pressure-induced amorphization breaking certain bonds17. In (MA)PbI3, the abrupt blueshift of the PL energy was ascribed to octahedral tilting, which decreases orbital overlapping19. For example, the blueshift of the PL energy under pressure has been observed in organolead perovskites17,19. For chalcopyrite ZnSiP2, Martinez et al.2 showed that SiZn2+ and/or PSi1+ antisite defects contribute to the donor level, while ZnSi2+ and/or SiP1- antisite defects form the acceptor level. The abnormal plateau could be attributed to the progressive development of cation disorder because donor–acceptor pair transitions are the primary PL mechanism in ZnSiP2. The optical micrographs in Fig. 2c demonstrate a piezochromic transition in compressed ZnSiP2. During the compression process, ZnSiP2 changes from its original transparent red to translucent dark red at 7.5 GPa and eventually turns to opaque black at 16.7 GPa.

Because of the insulating nature of ZnSiP2, the resistance at 300 K is beyond our instrumental limit (10Ω) and could not be detected below 14.0 GPa. Figure 3a shows the temperature dependence of the resistance R(T) of ZnSiP2 at various pressures up to 55.5 GPa. Starting from 14.0 to 21.5 GPa, ZnSiP2 displays semiconducting behavior, as evidenced by the increase in resistance upon cooling. A further increase in pressure leads to a semiconducting-metallic transition at 24.6 GPa. Strikingly, the occurrence of metallization is accompanied by a resistance drop below ~8.2 K (see Fig. 3b). The drop in the R(T) curve becomes increasingly sharper, and zero resistance is finally observed at 37.1 GPa, signaling pressure-induced superconductivity in ZnSiP2. Meanwhile, the superconducting critical temperature Tc decreases with increasing applied pressure, reaching a minimum at 37.1 GPa, followed by a continuous increase up to 55.5 GPa, the highest pressure applied in this study. We further measured the R(T) curves under various magnetic fields to determine the upper critical field at 44.4 GPa, as shown in Fig. 3c. By defining Tc as the onset temperature of the superconducting transition, we constructed the temperature-magnetic field phase diagram in the inset of Fig. 3c. According to the Wertheim–Helfand–Hohenberg (WHH) model35, the yielded upper critical field μ0Hc2(0) is ~3.0 T. Note that the upper critical field is much lower than the resultant Pauli limiting field of μ0Hc2(0) = 1.84Tc, which suggests the absence of Pauli pair breaking.
To obtain a comprehensive understanding of the evolution of the PL, electrical conductivity, and crystal structure in pressurized ZnSiP$_2$, we constructed a phase diagram, as shown in Fig. 4. It is clear that the appearance of superconductivity can be directly attributed to the structural transition from the tetragonal to cubic phase ca. 23 GPa. In the tetragonal phase, ZnSiP$_2$ is situated in the semiconducting regime but possesses the characteristic of cation disorder. As a prelude of the structural transition, the disorder in the cation sublattice gradually develops during compression, leading to the plateau present from 1.4 to 8.7 GPa in the pressure evolution of the PL peak energy. Along with the structural transition above ca. 23 GPa, ZnSiP$_2$ evolves into the superconducting regime. In agreement with the coexistence of tetragonal and cubic phases between 23 and 37 GPa, a measurable resistance is still observed at temperatures below the sharp resistance drop. Compared with the XRD results of Bhadram et al., who used Ar and He as PTMs, the coexisting pressure range is much larger in our case, which indicates that the coexistence of the two structures can be attributed not only to the incompleteness of the phase transition itself but also to the nonhydrostatic conditions. In the cubic phase, the superconducting phase diagram features an abnormal V-shaped evolution of $T_c$. We note that a similar V-shaped $T_c(P)$ behavior was previously reported in some superconducting compounds, such as AFe$_2$As$_2$.  

Fig. 3 Experimental evidence of pressure-induced superconductivity in ZnSiP$_2$. a Selective temperature-resistance curves $R(T)$ of ZnSiP$_2$ single crystals under compression. Inset: $R(T)$ curves in the range of 10–100 K. b Low-temperature $R(T)$ curves around the superconducting transition. The curve at 24.6 GPa is multiplied by 0.5 for comparison. c $R(T)$ curves under various magnetic fields at 44.4 GPa. Inset: Temperature-dependent upper critical field $\mu_0H_c$ at 44.4 GPa. The solid line represents the fitting based on the WHH model. Here, the $T_c$ value was defined as the onset temperature of the superconducting transition.

Fig. 4 Pressure evolution of the structural, optical, and electronic properties of ZnSiP$_2$. Pressure evolution of the superconducting transition onset temperature $T_c$ and PL peak energy from PL analyses. The colored areas are guides to the eyes, indicating the distinct conducting states, i.e., semiconductor, metal, and superconductor. The black and red horizontal arrows indicate the low-pressure tetragonal phase and high-pressure cubic phase, respectively.
(A = K, Rb, Cs)36,37, PbTaSe2,38, and TlInTe2,39, while the underlying mechanism is still under debate. On the one hand, the origin of V-shaped $T_c$ behavior has been discussed in terms of a change in the superconducting pairing symmetry or a Lifshitz transition across the critical pressure36,38. On the other hand, Yesudas et al.39 observed unusual giant phonon softening ($A_g$ mode) concomitant with the V-shaped $T_c(P)$ behavior in TlInTe2. In our case, one can see that the structural phase transition from the tetragonal to cubic phase is almost complete around the valley pressure of 36.7 GPa, which implies that the V-shaped behavior might be associated with abnormal evolution of the electron-phonon coupling due to the incompleteness of the phase transition in that pressure regime and/or to the nonhydrostatic conditions.

Conclusions
In summary, by systematically investigating the pressure effect on the optical and electronic properties, we demonstrate the pressure-induced abnormal evolution of the PL spectrum as well as superconductivity in the chalcopyrite semiconductor ZnSiP2. The abnormal evolution of the PL peak energy is accompanied by a piezochromic phenomenon relative to the structural phase transition from the tetragonal to cubic phase ca. 23 GPa. Based on the fact that a material with optoelectronic and photovoltaic applications is transformed into a superconductor, these findings provide crucial insight into the structure–property relationships in chalcopyrite semiconductors.

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Conflict of interest
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References
1. Li, W. et al. A new family of cation-disordered Zn(Cu–Si–P) compounds as high-performance anodes for next-generation Li-ion batteries. Energy Environ. Sci. 12, 2296–2297 (2019).
2. Martinez, A. D. et al. Solar energy conversion properties and defect physics of ZnSnP2. Energy Environ. Sci. 9, 1031–1041 (2016).
3. Medvedkin, G. A. & Voevodin, V. G. Magnetic and optical phenomena in nonlinear optical crystals ZnGeP2 and CdGeP2. J. Opt. Soc. Am. B 22, 1884 (2005).
4. He, G., Rozahn, J., Li, Z., Zhang, J. & Lee, M.-H. Size effect and identified superior functional units enhancing second harmonic generation responses on the II–IV–V2 type nonlinear optical crystals. Chem. Phys. 518, 101–106 (2019).
5. Martinez, A. D. et al. Development of ZnSnP2 for Si-based tandem solar cells. IEEE J. Photovolt. 5, 17–21 (2015).
6. Scanlon, D. O. & Walsh, A. Bandgap engineering of ZnSnP2 for high-efficiency solar cells. Appl. Phys. Lett. 100, 251911 (2012).
7. Sreepanvathy, P. C., Kanchana, V. & Vaithheeswaran, G. Thermoelectric properties of zinc based pnictide semiconductors. J. Appl. Phys. 119, 085701 (2016).
8. Liu, R. et al. High-throughput screening for advanced thermoelectric materials: diamond-like ABX3 compounds. ACS Appl. Mater. Interfaces 11, 24859–24866 (2019).
9. Shaj, J. L., Teli, B., Buehler, E. & Wernick, J. H. Band structure of ZnGeP2 and ZnSnP2—ternary compounds with pseudodirect energy gaps. Phys. Rev. Lett. 30, 983–986 (1973).
10. Sadhukhan, B., Zhang, Y., Ray, R. & van den Brink, J. First-principles calculation of shift current in chalcopyrite semiconductor ZnSnP2. Phys. Rev. Mater. 4, 064602 (2020).
11. Martinez, A. D., Fioretti, A. N., Toberer, E. S. & Tamboli, A. C. Synthesis, structure, and optoelectronic properties of II–IV–V2 materials. J. Mater. Chem. A 5, 11418–11435 (2017).
12. Martinez, A. D. et al. Growth of amorphous and epitaxial ZnSnP2–Si alloys on Si. J. Mater. Chem. C 6, 2696–2703 (2018).
13. Liu, H. et al. The pressure-effects on phase transitions, band structures, electronic and elastic properties of ternary compounds ZnX2P2 (X = Si, Ge, Sn) by first principle calculations. Mater. Res. Express 5, 126303 (2018).
14. Zhang, L. et al. Pressure-induced emission enhancement, band-gap narrowing, and metalization of halide perovskite Cs6Bi5I23. Angew. Chem. Int. Ed 57, 11213–11217 (2018).
15. Yuan, Y. et al. Large band gap narrowing and prolonged carrier lifetime of (C4H9NH3)2PbI4 under high pressure. Adv. Sci. 6, 1900240 (2019).
16. Liang, Y. et al. New metallic ordered phase of perovskite Cs3Bi2I9. J. Mater. Chem. C 6, 9830–9834 (2018).
17. Wang, Y. et al. Pressure-induced phase transformation, reversible amorphization, and anomalous visible light response in organolead bromide perovskite. J. Am. Chem. Soc. 137, 11144–11149 (2015).
18. Liu, G. et al. Pressure-induced bandgap optimization in lead-based perovskites with prolonged carrier lifetime and ambient reactivity. Adv. Funct. Mater. 27, 1604208 (2017).
19. Jaffe, A. et al. High-pressure single-crystal structures of 3D lead-halide hybrid perovskites and pressure effects on their electronic and optical properties. ACS Cent. Sci. 2, 201–209 (2016).
20. Chi, Z. et al. Superconductivity in pristine 2H$_2$MoS$_2$ at ultrahigh pressure. Phys. Rev. Lett. 120, 037002 (2018).
21. Zhou, Y. et al. Pressure-induced metallization and robust superconductivity in pristine 1T-SnSe$_2$. Adv. Electron. Mater. 4, 1800155 (2018).
22. Badram, V. S. et al. Pressure-induced structural transition in chalcopyrite ZnSiP$_2$. Appl. Phys. Lett. 110, 182106 (2017).
23. Arab, F., Sahraoui, F. A., Haddadi, K. & Louai, L. Ab initio investigations of structural, elastic and electronic properties of ZnSiP$_2$. Pressure effect. Comp. Mater. Sci. 65, 520–527 (2012).
24. Spring-Thorpe, A. J. & Pamplin, B. R. Growth of some single crystal II–IV–V$_2$ semiconducting compounds. J. Cryst. Growth 3–4, 313–316 (1968).
25. Prescher, C. & Prakapenka, V. B. DIOPTAS: a program for reduction of two-dimensional X-ray diffraction data and data exploration. High. Press. Res. 35, 223–230 (2015).
26. Hunter, B. A. Rietica—A Visual Rietveld Program, International Union of Crystallography Commission on Powder Diffraction Newsletter No. 20, http://www.rietica.org, (1998).
27. Mao, H. K., Xu, J. & Bell, P. M. Calibration of the ruby pressure gauge to 800 kbar under quasi-hydrostatic conditions. J. Geophys. Res. 91, 4673–4676 (1986).
28. Gontijo, R. N. et al. Temperature dependence of the double-resonance Raman bands in monolayer MoS$_2$. J. Raman Spectrosc. 50, 1867–1874 (2019).
29. Dey, P. et al. Optical coherence in atomic-monolayer transition-metal dichalcogenides limited by electron-phonon interactions. Phys. Rev. Lett. 116, 127402 (2018).
30. Birch, F. Finite elastic strain of cubic crystals. Phys. Rev. 71, 809–824 (1947).
31. Peña-Pedraza, H., López-Rivera, S. A., Martin, J. M., Delgado, J. M. & Power, C. Crystal and phonon structure of ZnSiP$_2$, a II-IV-V$_2$ semiconducting compound. Mater. Sci. Eng. B 177, 1465–1469 (2012).
32. Bernard, J. E. & Zunger, A. Ordered-vacancy-compound semiconductors: pseudocubic CdIn$_2$Se$_4$. Phys. Rev. B 837, 6835–6856 (1988).
33. Zunger, A. Order-disorder transformation in ternary tetrahedral semiconductors. Appl. Phys. Lett. 50, 164–166 (1987).
34. Burlakov, I. I., Raptis, Y., Ursaki, V. V., Anastassakis, E. & Tiginyanu, I. M. Order-disorder phase transition in CdAl$_2$S$_4$ under hydrostatic pressure. Solid State Commun. 101, 377–381 (1997).
35. Wemhöner, N. R., Helfand, E. & Hohenberg, P. C. Temperature and purity dependence of the superconducting critical field, $H_{c2}$ III. electron spin and spin-orbit effects. Phys. Rev. 147, 295–302 (1966).
36. Tafti, F. F. et al. Sudden reversal in the pressure dependence of $T_c$ in the iron-based superconductor KFe$_2$As$_2$. Nat. Phys. 9, 349–352 (2013).
37. Tafti, F. F. et al. Sudden reversal in the pressure dependence of $T_c$ in the iron-based superconductor CsFe$_2$As$_2$: a possible link between inelastic scattering and pairing symmetry. Phys. Rev. B 89, 134502 (2014).
38. Pang, G. M. et al. Nodeless superconductivity in noncentrosymmetric PbTaSe$_2$ single crystals. Phys. Rev. B 93, 060506(R) (2016).
39. Yesudhas, N. Y. S. et al. Origin of superconductivity and giant phonon softening in TIlTe$_2$ under pressure. Preprint at https://arxiv.org/abs/2003.09604 (2020).