Abstract
Thermoelectric properties of single crystal Ta$_2$PdSe$_6$ is investigated by means of transport measurements, and a density functional calculation. We found a giant Peltier conductivity of 100 A cm$^{-1}$ K$^{-1}$ at 10 K and successfully explained it by means of conventional semiconductor theory. We concluded that an uncompensated semimetal, high mobility, and heavy effective mass are responsible for the giant Peltier conductivity. Our finding opens a new ground in the field of thermoelectrics to explore much better semimetals for a new possible application such as an electric current generator for a superconducting magnet.

1. Introduction
Itinerant electrons in solids in a thermal equilibrium are driven not only by an external electric field, but also by a temperature gradient $\nabla T$, and form a steady flow, i.e. an electrical current density $j$. While the former case is known as Ohm's law, the latter is rather recognized as the origin of the Seebeck effect that an electric field is generated by $\nabla T$ in an open circuit. In fact, Ohm used $j$ generated $\nabla T$ to find Ohm's law. The proportionality constant between $j$ and $\nabla T$ has been called the Peltier conductivity $P$ as $j = P(-\nabla T)$. Despite many studies for thermoelectrics, a theoretical upper limit of $P$ has yet to be explored, and accordingly an unexpectedly large $P$ has a great potential to revolutionize modern electronics.

Here, we report the observation of a giant $P$ of 100 A cm$^{-1}$ K$^{-1}$ at 10 K in a single crystal of the layered semimetal Ta$_2$PdSe$_6$ [1]. This value is 200 times larger than the maximum $P$ of the commercially available thermoelectric material Bi$_2$Te$_3$ [2, 3], and, to the best of our knowledge, it is the largest ever reported for a bulk material. This value may open a novel heat-to-electricity conversion such as a current generator, in which a 1 cc sample generates an electric current of 100 A with a temperature difference of 1 K. This is applicable to an isolated current source set in a cryogenic space. Using a two-carrier model for a perfectly uncompensated semimetal, we clarified why and how such a giant value is realized in the title compound.

2. Method
High-quality single crystals of Ta$_2$PdSe$_6$ were grown by means of $I_2$ vapor transport. Powders of tantalum (99.9%), palladium (99.9%), and selenium (99.9% or 99.999%) were loaded into an evacuated quartz tube with a $I_2$ concentration of $\sim$3 mg cm$^{-3}$. Then, a temperature difference of 145 °C between 875 °C and 730 °C in a three-zone furnace was used for crystal growth for four days. Single phase polycrystalline sample was synthesized using the same starting powder. Once the raw powder was heated up to 550 °C, then the re-grinded powder was heated at 730 °C for 48 h in a tube furnace.

Ta$_2$PdSe$_6$ crystals were chemically characterized by scanning electron microscopy with energy dispersive x-ray spectroscopy (JEOL JSM-7500F). The ratio of Ta:Pd:Se was evaluated to be 1.91:0.93:6.14, which agrees with the stoichiometric ratio of Ta$_2$PdSe$_6$ (figure S1 (available online at stacks.iop.org/JPENERGY/3/044004/mmedia)). We also conducted a synchrotron single crystal x-ray diffraction (XRD) measurement at BL02B1.
in SPring-8. We employed a wavelength of 0.30963 Å to obtain a high-resolution data. We used a gas-blowing device for sample temperature control, and a Pilatus3 X 1M CdTe detector [5] for measuring two-dimensional diffraction patterns (figure S2). Diffraction intensity averaging was performed using SORAV [5], and crystal structure refinement was performed by means of the SHELX least squares program [6]. The refined ratio of Ta and Se against Pd was 1.997 and 5.998 respectively, indicating the atomic deficiency is less than 1%. A summary of the structural analysis is provided in tables 1 and S1.

Transport properties, including electrical resistivity, thermopower, and Hall resistivity, were measured using a physical property measurement system (PPMS) (Quantum Design). The electrical resistivity was measured along the b axis by a four-probe method using gold wires with 20 μm diameters and the silver paste. The thermopower along the b axis was measured with a steady state and the two-probe technique. The sample bridged two separated copper heat baths, and the resistance heater (KYOWA KFLB-02-120-C1-11) created a temperature difference between the two heat baths, which was monitored through a copper-constantan differential thermocouple. The contribution of the voltage leads was carefully subtracted. The Hall resistivity with the four-probe technique was achieved by sweeping an out-of-plane magnetic field from −4 to 4 T with a steady current along the b axis. The typical setup for the transport measurements is shown in figure S3. The resistivity at each magnetic field were collected using ΔR mode of a nano-ohmmeter LR-700 (Linear Research Inc.). The Hall resistivity ρxy was obtained by calculating (ρxy(+H) − ρxy(−H))/2.

The specific heat measurements were performed by relaxation method with a commercial measurement system (Quantum Design PPMS Dynacool) by using polycrystalline Ta6PdSe6. The heat capacity was measured from 3 K to 300 K.

The band structure calculations were performed using the pseudopotential method based on the projector augmented wave formalism [7] with plane-wave basis sets implemented in Quantum Espresso (version 6.6) [8]. The cut-off energies for plane waves and charge densities were set to 44 and 448 Ry in the full relativistic calculations. We conducted structure optimization using the structural parameter obtained from the single crystal XRD at 100 K as an initial input. We used a 14×14×4 uniform k-point mesh with the cold smearing method during self-consistent loops and 30×30×10 points with the ‘tetrahedra_opt’ method for density-of-states and Fermi-surface calculation. Figure S4 shows the orbital-resolved Fermi surface.

3. Result and discussion

The Peltier conductivity P can be understood from the Seebeck effect, in which a voltage difference of ΔV is generated across a sample subjected to a temperature difference of ΔT. The proportionality constant S is called the Seebeck coefficient, and ΔV = SΔT. In the presence of ΔT, materials can behave like a battery with an open circuit voltage of ΔV and an internal resistance of the sample R, as schematically shown in the inset of figure 1. In case the load resistance is much smaller than R, the maximum thermoelectric current is calculated to be (ΔV/R), from which P is evaluated as V/Sρ as a parameter intrinsic to materials, where ρ is the resistivity. Figure 1(a) shows |P| of various materials [9] plotted as a function of conductivity σ = 1/ρ. We can find that Ta6PdSe6 locates at the top-level even at 300 K, and the highest at 10 K among the thermoelectric materials.

Figure 1(b) shows a comparison of the temperature dependence of |P| between Ta6PdSe6 and other representative low- and middle-temperature thermoelectric materials [10–14]. We find that |P| of others except for YbAgCu4 takes at most of the order of 1 A cm⁻¹ K⁻¹, and gradually decreases as temperature decreases. Since optimized thermoelectric materials show a substantial residual resistivity accompanied by the T-linear S at low temperatures, their |P| is expected to be linear in T at low temperatures. On contrary, |P| of Ta6PdSe6 rapidly increases below 100 K to reach a giant value of 100 A cm⁻¹ K⁻¹ at 10 K, indicating the giant P results from an extremely low residual resistivity.

We show ρ and S of single-crystal Ta6PdSe6 plotted as a function of temperature in figures 2(a) and (b), respectively. The two quantities are measured along the longitudinal dimension (the b axis shown in figures 3(a) and (b)) of a needle-like single crystal, shown in the inset of figure 2(a). The resistivity ρ reaches a low value of 10⁻⁷ Ω cm at 2 K with a residual resistance ratio (RRR) of 694. This RRR value is much better than that of other chalcogenide semimetals [15, 16]. S takes a relatively large value of 40 μV K⁻¹ at 20 K. Consequently, the calculated P result in the giant value of 100 A cm⁻¹ K⁻¹ at 10 K as shown in figure 2(c). Note that the power factor, which is a measure of electric power of the sample subjected to a temperature difference of 1 K, also becomes a huge value of 2.4 mW cm⁻¹ K⁻² at 15 K, although we previously reported a relatively large value of 13 μW cm⁻¹ K⁻² at 300 K [17]. We also pointed out this compound is semimetallic, for S shows a sign change near 100 K. These trends are well reproduced between different single crystals (see figures S5(a) and (b)).
We should point out that the contribution of the phonon drag effect to $S$ is negligible in Ta$_2$PdSe$_6$. As shown in figure S5, the single crystal prepared by using low-purity (99.9%) selenium powder shows worse conductivity than that prepared by high-purity (99.999%) selenium powder at the lowest temperature. This indicates that the carriers are scattered more frequently by the introduced impurities in the low-purity sample. Nevertheless, $S$ of the low-purity sample is almost the same as the high-purity one. If the phonon drag effect effectively contributed to $S$, $S$ would have to be affected by the impurity doping, since the mean free path of phonons is generally longer than that of electrons. This proves that the phonon drag effect is negligible and the diffusive part of electrons mainly contributes to $S$ of Ta$_2$PdSe$_6$. 

Figure 1. Comparison of the Peltier conductivity $|P|$ between Ta$_2$PdSe$_6$ and other thermoelectric materials. (a) $|P|$ for a wide variety of materials plotted against electrical conductivity ($1/\rho$). The data points except for Ta$_2$PdSe$_6$ are obtained from the Materials Research Laboratory database [9] of 300 K. (b) Temperature dependence of $|P|$ for Ta$_2$PdSe$_6$, Bi$_2$Te$_3$ [10], Na$_{0.88}$CoO$_2$ [11], Ta$_4$SiTe$_4$ [12], YbAgCu$_4$ [13], and CsBi$_4$Te$_6$ [14].
Figure 2. Electrical transport properties of Ta$_2$PdSe$_6$. (a) Temperature dependence of electrical resistivity ($\rho$), showing high conductivity at low temperature. The inset shows a photographic image of a single crystal. (b) Temperature dependence of thermopower ($S$). Note that the sign changes around 100 K. (c) Temperature dependence of the Peltier conductivity and power factor ($= S\sigma$).

Figures 3(a) and (b) shows the crystal structure of layered selenide Ta$_2$PdSe$_6$, the layers of which consist of face-shared TaSe$_6$ prisms and square-planar PdSe$_4$. The crystal structure is visualized by VESTA [18]. Ta$_2$PdSe$_6$ was first synthesized in 1985, and its electric resistivity was investigated [1]. Ta$_2$PdSe$_6$ has a structural similarity to the excitonic insulator candidate Ta$_2$NiSe$_5$ [19], a material in which we found unique structural [20, 21] and transport properties [22, 23]. Thus, we focused on Ta$_2$PdSe$_6$ as a related material and then identified the giant Peltier conductivity.

We now take a closer look at the electronic states of Ta$_2$PdSe$_6$. Before a band structure calculation, we performed a structural optimization to obtain a lowest-temperature structure by starting from a crystal structure determined by a synchrotron single-crystal XRD measurement at 100 K (table 1). The relaxed lattice and atomic coordination parameters are listed in table 2. Figures 3(c) and (e) shows the Fermi surface visualized by FermiSurfer [24] and band dispersion around the Fermi energy ($E_F$) along the MCLC$_1$ path [25]. There is an electron Fermi surface near the I, X, and N points, while a hole Fermi surface near the $\Gamma$, Y, L, and Z points, indicating a semimetallic ground state. Figure 3(f) shows the total and partial density of states, demonstrating that Ta 5d and Se 4p components mainly contribute to the low-energy electronic states. This is also shown by the orbital-resolved Fermi surface in figure 4. The calculated Fermi surface in figure 3(c) is shaped like a ragged, corrugated plane perpendicular to the b axis, indicating a pseudo one-dimensional (1D) electronic structure.

Now we explain how the giant $P$ realized in terms of a two-carrier model [26]. The partial conductivities of the electron ($\sigma_e$) and hole ($\sigma_h$) can be written as

$$\sigma_e = 2ne\mu_e,$$

(1)
Figure 3. Crystal and electronic structure of Ta$_2$PdSe$_6$. (a) The layered crystal structure of Ta$_2$PdSe$_6$ viewed from the b axis. (b) The intra-layer structure viewed from the stacking direction (the visualization software is VESTA [18]). Each layer includes two types of one-dimensional chains, consisting of square-planar PdSe$_4$ and face-shared TaSe$_6$ prisms which stack and extend along the b axis. (c) Fermi surface of Ta$_2$PdSe$_6$ (the Fermi surface is visualized by FermiSurfer [24]). (d) High symmetry points of the Brillouin zone. (e) Band structure calculation along the MCLC$_1$ path, demonstrating a semimetallic ground state of Ta$_2$PdSe$_6$. (f) Density of state (DOS) around the Fermi energy ($E_F$). The partial DOS for Ta 5d, Pd 4d, and Se 4p orbitals are also shown.

Table 1. Refined structural parameters for Ta$_2$PdSe$_6$ at 100 K determined by single crystal synchrotron x-ray diffraction. The space group is C$2/m$, and the obtained lattice parameters are $a = 12.4179(3)$ Å, $b = 3.3691(1)$ Å, $c = 10.3951(3)$ Å, and $\beta = 116.192(8)^\circ$. The number of unique reflections for the refinement within the resolution limit $d > 0.3$ Å is 34 192. The obtained $R$ factor and GOF are 3.36% and 1.047%, respectively.

| Atom  | Site | x    | y    | z    | $B_{eq}$ (Å$^2$) |
|-------|------|------|------|------|-----------------|
| Ta    | 4$m$ | 0.67992(2) | 0    | 0.28974(2) | 0.1059(8) |
| Pd    | 2$a$ | 1/2  | 1/2  | 0    | 0.2258(16) |
| Se(1) | 4$m$ | 0.71915(2) | 1/2  | 0.12513(2) | 0.1808(16) |
| Se(2) | 4$m$ | 0.50566(2) | 1/2  | 0.23897(2) | 0.1713(16) |
| Se(3) | 4$m$ | 0.84156(2) | 1/2  | 0.46069(2) | 0.1555(16) |
Thus, we conclude that the lightly doped holes with high mobility and heavy mass are responsible for the giant Peltier effect, which is well defined by

$$S = \frac{\sigma_e S_e + \sigma_h S_h}{\sigma_e + \sigma_h}.$$  

Using equations (5)–(7), we get

$$S(f) = \frac{\alpha_0 p^{-2} T (\rho m_h - 4 (1 - f) m_e)}{4}.$$  

To find $p$, $m_h$, and $f$, we measured the Hall resistivity $\rho_{xy}$ at various temperatures, as shown in figure 4(a). Little deviation from linear-field dependence implies that $R_{HI}$ is well defined by $p_{xy}/\mu_0 H$ at 1 T. $R_{HI}$ clearly shows a rapid decrease from $10^{-2}$ down to $10^{-3}$ cm$^2$V$^{-1}$s$^{-1}$ around 100 K, as shown in figure 4(b). Assuming a heavily uncompensated condition of $f \approx 1$ at 2 K, we obtain $p \approx 7 \times 10^{20}$ cm$^{-3}$ from equation (4), which is roughly consistent with the calculated carrier concentration of $7.5 \times 10^{20}$ cm$^{-3}$. We also evaluate $\mu_0$ at 2 K to be $9 \times 10^4$ cm$^2$V$^{-1}$s$^{-1}$ from $R_{HI}/\rho$. Furthermore, using equation (9), we get $m_h = 2.9 m_0$ ($m_0$ is the bare electron mass) for $S = 40 \mu$V K$^{-1}$ and $T = 20$ K. This value is roughly consistent with the effective mass of 3.5$m_0$ estimated from the electron specific heat coefficient $\gamma$ and $n$ (see table 3 and figure S6). Thus, we conclude that the lightly doped holes with high mobility and heavy mass are responsible for the giant Peltier conductivity in Ta$_2$PdSe$_6$.

In the field of thermoelectrics, the so-called B-factor is a measure of good thermoelectric materials [27]. It is proportional to $(m^*)^{3/2} \mu / \kappa_L$, where $m^*$, $\mu$, and $\kappa_L$ are the effective mass, the mobility, and the lattice thermal conductivity of a material, respectively. The numerator $(m^*)^{3/2} \mu$ characterizes the power factor and is 4000 times larger for Ta$_2$PdSe$_6$ than for Bi$_2$Te$_3$ ($m^* = 0.2 m_0$ and $\mu = 1200$ cm$^2$V$^{-1}$s$^{-1}$). This is indicative of the large power factor in the present compound (2.4 mW cm$^{-1}$ K$^{-2}$ at 15 K). The 1D electronic structure plays a vital role to achieve such high $(m^*)^{3/2} \mu$, since light holes along the 1D direction are responsible for the high mobility, whereas holes perpendicular to the 1D direction are responsible for the heavy mass [28].

### Table 2. Relaxed structural parameters for Ta$_2$PdSe$_6$. The space group is $C2/m$, and the lattice parameters are $a = 12.3296$ Å, $b = 3.34581$ Å, $c = 10.3233$ Å, and $\beta = 116.157^\circ$.

| Atom | Site | $x$   | $y$   | $z$   |
|------|------|-------|-------|-------|
| Ta   | 4m   | 0.67830 | 0     | 0.28743 |
| Pd   | 2a   | 1/2    | 1/2   | 0     |
| Se(1) | 4m  | 0.72160 | 1/2   | 0.12404 |
| Se(2) | 4m  | 0.50348 | 1/2   | 0.24021 |
| Se(3) | 4m  | 0.84163 | 1/2   | 0.46061 |

$$\sigma_h = p e \mu_h,$$

where $n (p)$, $e$, and $\mu_{e(h)}$ are the concentration of electrons (holes) per valley, the element charge, and the carrier mobility of the electron (hole), respectively. Note that the factor of two in $\sigma_e$ represents the valley degeneracy. Then, the net Hall coefficient $R_{HI}$ is described as

$$R_{HI} = \frac{p \mu_h^2 - 2 n \mu_e^2}{e (p \mu_h + 2 n \mu_e)}.$$  

Imposing a semimetallic condition of $2n = p$, we rewrite equation (3) as

$$R_{HI} (f) = \frac{1}{pe} (2f - 1),$$  

where $f = \mu_p / (\mu_h + \mu_e)$. For pseudo 1D parabolic bands, the partial thermopowers of electron ($S_e$) and hole ($S_h$) are given by (see supporting information)

$$S_e = -\alpha_0 m_e (p/2)^{-2} T,$$

$$S_h = \alpha_0 m_h p^{-2} T,$$

$$\alpha_0 = \frac{A^2 k_B^2}{4 \pi^2 e h^2},$$

where $k_B$, $h$, $m_{e(h)}$, and $A$, are the Boltzmann constant, the Planck constant, the effective mass of electrons (holes), and the cross-section of the Brillouin zone perpendicular to the $b$ axis, respectively. The net thermopower is given by

$$S = \frac{\sigma_e S_e + \sigma_h S_h}{\sigma_e + \sigma_h}.$$  

Using equations (5)–(7), we get

$$S(f) = \frac{\alpha_0 p^{-2} T (\rho m_h - 4 (1 - f) m_e)}{4}.$$  

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Figure 4. Magnetic transport properties of Ta$_2$PdSe$_6$. (a) Hall resistivity $\rho_{yx}$ at various temperatures. (b) Temperature dependence of Hall coefficient ($R_H$). The dotted line shows $2f-1$ calculated using the measured $S$ data (see text).

Table 3. Comparison of evaluated carrier concentration ($n$), electron specific coefficient ($\gamma$), and carrier effective mass ($m^*$) between the experiment and DFT calculation. $m_0$ is the bare electron mass.

|                | Exp.        | Calc.                                      |
|----------------|-------------|--------------------------------------------|
| $n$ (cm$^{-3}$) | $7 \times 10^{20}$ (hole) | $7.5 \times 10^{20}$ (hole, assuming $n=p$) |
| $\gamma$ (mJ mol$^{-1}$ K$^{-2}$) | 6.4 | 4.2 |
| $m^*$          | 2.9$m_0$ (Seebeck) | 0.4$m_0$ ($k \parallel b$) |
|                | 3.5$m_0$ (specific heat) | 2.2$m_0$ ($k \perp b$) |

also note that Ta$_2$PdS$_6$, an isostructural compound of Ta$_2$PdSe$_6$, shows relatively high power factor $\sim 30 \, \mu$W cm$^{-1}$ K$^{-2}$ at 300 K [17].

At higher temperatures, the electron conduction begins to contribute. Since we have determined $p$ and $m_h$ already, only $m_e$ is left as an unknown parameter in equation (9). Setting $m_e = 0.9m_0$ as an adjustable parameter, we obtain $f$ from the measured $S$ though equation (9). In figure 4(b), we show the thus-obtained $2f-1$, which reasonably matches with $R_H(f)$. In short, all the measured transport parameters are quantitatively and consistently understood in terms of low carrier concentration, heavy mass, high hole mobility, and a crossover from $f=1/2$ (compensated) to $f \sim 1$ (heavily uncompensated).

The giant Peltier conductivity and huge power factor can be used as a current source for a superconducting solenoid isolated in a cryogenic space. For 100 A cm$^{-1}$ K$^{-1}$, a cubic sample of 1 cc would supply a thermoelectric current of 100 A to the zero-resistance solenoid for a temperature difference of 1 K. An absence of external current leads can make the system compact and concise and reduce cooling costs for such a solenoid. This can be a novel application of heat-to-electricity conversion. We notice that the induction voltage can be larger than $S\Delta T$, so that the field-sweeping rate must be kept low.

Our finding suggests that uncompensated semimetals can generate substantial electricity at low temperatures. This type of application will break new ground in the field of thermoelectrics. Semimetals are of high mobility in general and show good electrical conduction without impurity doping [29]. The uncompensated condition of $f \sim 1$ partly comes from electron–hole asymmetry as shown in figure 3(c), and ternary or quaternary compounds may satisfy this condition. Such materials have never been researched, and therefore we believe that much better semimetals exist but are to date unknown.

Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

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ORCID iDs

Akitoshi Nakano https://orcid.org/0000-0001-9780-5179
Hiroti Taniguchi https://orcid.org/0000-0002-1773-7856
Ichiro Terasaki https://orcid.org/0000-0002-6073-2639

References

[1] Keszler D A, Squatrito P J, Brese N E, Ibers J A, Shang M and Lu J 1985 Ta₃PdS₆, Ta₃PdSe₆, Nb₂PdS₆, Nb₂PdSe₆ Inorg. Chem. 24 3065–7
[2] Bos J W, Zandbergen H W, Lee M-H, Ong N P and Cava R J 2007 Structural and thermoelectric properties of the infinitely adaptive series (Biₓ,Snₓ)(Bi₄Te₁₀) In. Phys. Rev. B 75 195203
[3] Satterthwaite C B and Ure R W 1957 Electrical and thermal properties of Bi₂Te₃ Phys. Rev. 108 1164
[4] Krause L, Tolborg K, Gronbech T B E, Sugimoto K, Iversen B B and Overgaard J 2020 Accurate high-resolution single-crystal diffraction data from a Pilatus3 X CdTe detector J. Appl. Crystallogr. 53 625
[5] Blessing R H 1987 Data reduction and error analysis for accurate single-crystal diffraction intensities Crystallogr. Rev. 1 3
[6] Sheddick G M 2015 Crystal structure refinement with SHEXL Acta Crystallogr. C71 3
[7] Blochl P E 1994 Projector augmented-wave method Phys. Rev. B 50 17953
[8] Paolo G et al 2009 Quantum Espresso: a modular and open-source software project for quantum simulations of materials J. Phys.: Condens. Matter. 21 395502
[9] Gaultois M W, Sparks T D, Borg C K H, Sheshadi R, Bonifício W D and Clarke D R 2013 Data-driven review of thermoelectric materials: performance and resource considerations Chem. Mater. 25 2911
[10] Hor Y S et al 2010 Low temperature magnetothermoelectric effect and magnetoresistance in Te vapor annealed Bi₂Te₃ J. Phys.: Condens. Matter 22 375801
[11] Lee M, Vicin L, Li L, Wang Y, Foo M L, Watauchi S, Pascal Jr R A, Cava R J and Ong N P 2006 Large enhancement of the thermopower in Na₂CoO₃ at high Na doping Nat. Mater. 5 537–40
[12] Inohara T, Okamoto Y, Yamakawa Y, Yamakage A and Takenaka K 2017 Large thermoelectric power factor at low temperatures in one-dimensional telluride Ta₃SIE₃ Appl. Phys. Lett. 110 183901
[13] Koirala M, Wang H, Pokharel M, Lan Y, Guo C, Opeil C and Ren Z 2014 Nanostructured YbCu₃As₃ for potentially cryogenic thermoelectric cooling Nano Lett. 14 5016–20
[14] Chung D Y et al 2000 CdBi₂Te₃—a high-performance thermoelectric material for low-temperature applications Science 287 1024
[15] Takahashi H, Akiba T, Imura K, Shinno T, Deguchi K, Sato N K, Sakai H, Bahrany M S and Ishiwata S 2017 Anticorrelation between polar lattice instability and superconductivity in the Weyl semimetal candidate MoTe₂ Phys. Rev. B 95 100501R
[16] He J et al 2017 Band dependence of charge density wave in quasi-one-dimensional Ta₃NiSe₆ probed by orbital magnetoresistance Appl. Phys. Lett. 111 052405
[17] Nakano A, Maruoka U, Kato F, Taniguchi H and Terasaki I 2021 Room temperature thermoelectric properties of isostructural selenides Ta₃PdS₆ and Ta₃PdSe₆ J. Phys. Soc. Japan 90 033702
[18] Izumi F and Momma K 2007 Three-dimensional visualization in powder diffraction Solid State Phenom. 130 15–20
[19] Lu Y F, Kono H, Larkin T I, Rost A W, Takayama T, Boris A V, Keimer B and Takagi H 2017 Zero-gap semiconductor to excitonic insulator transition in Ta₃NiSe₆ Nat. Commun. 8 14408
[20] Nakano A et al 2018 Pressure-induced coherent sliding-layer transition in the excitonic insulator Ta₃NiSe₆ IUCrJ 5 158
[21] Nakano A, Hasegawa T, Tamura S, Katayama N, Tsutsui S and Sawa H 2018 Antiferroelectric distortion with anomalous phonon softening in the excitonic insulator Ta₃NiSe₆ Phys. Rev. B 98 045139
[22] Nakano A, Nagai T, Katayama N, Sawa H, Taniguchi H and Terasaki I 2019 Exciton transport in the electron–hole system Ta₃NiSe₆ J. Phys. Soc. Japan 88 113706
[23] Nakano A, Maruoka U, Taniguchi H and Terasaki I 2020 Examination of nonlinear conductivity on the excitonic insulator candidate Ta₃NiSe₆ J. Phys. Soc. Japan 89 045001
[24] Kawamura M 2019 FermiSurfer: Fermi-surface viewer providing multiple representation schemes Comput. Phys. Commun. 239 197
[25] Setyawan W and Curtarolo S 2010 High-throughput electronic band structure calculations: challenges and tools Comput. Mater. Sci. 49 299
[26] Klein Y and Terasaki I 2007 Transport properties of the quasi-one-dimensional barium ruthenates Phys. Rev. B 73 165105
[27] Mahan G D 1989 Figure of merit for thermoelectrics J. Appl. Phys. 65 1578
[28] Shirai K and Yamanaka K 2013 Mechanism behind the high thermoelectric power factor of SrTiO₃ by calculating the transport coefficient J. Appl. Phys. 113 053705
[29] Markov M et al 2019 Thermoelectric properties of semimetals Phys. Rev. Mater. 3 095401