

Origin of the absence of a charge density wave in the kagome metal TiV_6Sn_6 : A rattling chain model–predicted AM_6X_6 -type charge density wave compound

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The rattling chain model has provided a useful phenomenological guideline for identifying AM_6X_6 -type kagome charge density wave (CDW) materials. In this work, we performed a comprehensive experimental and theoretical investigation of TiV_6Sn_6 , a kagome CDW material predicted by the rattling chain model. However, resistivity, magnetization, and specific heat measurements reveal no evidence of a CDW transition in TiV_6Sn_6 . Furthermore, unlike its rare-earth-based sister compound $RV_6\text{Sn}_6$ ($R = \text{Sc}, \text{Y}, \text{Sm}, \text{and Gd-Lu}$), phonon calculations show that TiV_6Sn_6 exhibits no imaginary phonon modes under either compressive or tensile strain. The band structure and crystal orbital Hamilton population (COHP) curves of TiV_6Sn_6 exhibit recognizable differences from those of $RV_6\text{Sn}_6$. Further analysis attributes these differences to the higher electronegativity of Ti relative to the rare-earth elements. The enhanced electronegativity promotes mixed ionic-covalent bonding, where the covalent character suppresses the rattling motion of Ti, ultimately precluding the formation of a CDW. Our findings suggest that the electronegativity of the filler atom, in addition to its ionic radius, should be incorporated as a supplementary factor into the rattling chain model.

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I. INTRODUCTION

Rational design of new materials has emerged as an important research frontier in recent years, enabling scientists to identify target materials based on simple chemical rules quickly. Recently, the charge density wave (CDW) in kagome materials has attracted intensive attention due to its intertwining with various orders such as superconductivity, nematic phase, or magnetism [1–7]. Substantial efforts have been devoted to exploring new kagome CDW materials, leading to empirical criteria such as the rattling chain model [8,9]. The rattling chain model predicts that the CDW in HfFe_6Ge_6 -structured AM_6X_6 materials originates from the rattling of an A - X - X - A chain residing in the hexagonal voids of the kagome and honeycomb layers [8,9]. Then the prerequisite for the occurrence of the CDW transition is sufficient space for the chain to rattle, i.e., a combination of the small atomic size of A atoms and the large size of the M_6X_6 host lattice [8]. The rattling chain model has provided a useful phenomenological guideline, which gives a plausible explanation to the existing AM_6X_6 -type CDW materials (ScV_6Sn_6) [8] and successfully predicts a new one (LuNb_6Sn_6) [10].

However, the rattling chain model primarily emphasizes the relative size between the filler atom and the corresponding void in the lattice, ignoring the bonding properties of the filler atom. Among the filler atoms in AFe_6Ge_6 ($A = \text{Li}, \text{Mg}, \text{Ti}, \text{Zr}, \text{Hf}, \text{Nb}, \text{Sc}, \text{Y}, \text{and Gd-Lu}$) materials [11–13], Ti possesses the smallest ionic radius. Following the prediction of the rattling chain model, TiFe_6Ge_6 would be expected to host the CDW. Contrary to this expectation, our experimental investigation on $\text{Ti}_{0.85}\text{Fe}_6\text{Ge}_6$ reveals no signature of a CDW transition. Meanwhile, the calculated electronic structure of TiFe_6Ge_6 differs significantly from that of FeGe and other AFe_6Ge_6 compounds [11]. Analysis of the band structure, density of states (DOS), and crystal orbital Hamilton population (COHP) suggests that the absence of CDW can be attributed to Ti's bonding characteristics, which differ significantly from those of rare-earth elements. Nevertheless, since the model's key prerequisite is not fully satisfied, where both Ti and the host lattice are small, the explanation based on the chemical bonding remains inconclusive [11]. Therefore, it is crucial to further verify the rattling chain model on a more qualified candidate material with a small filler atom but a large host lattice.

According to the phase diagram of cell volume versus the A -site VIII-coordination Shannon radius reported by Ortiz *et al.* [see Fig. 1(c) in Ref. [10]], only four compounds— TiV_6Sn_6 , ZrV_6Sn_6 , HfV_6Sn_6 , and ScV_6Sn_6 —fall within the region predicted to exhibit CDW order. Experimentally, the

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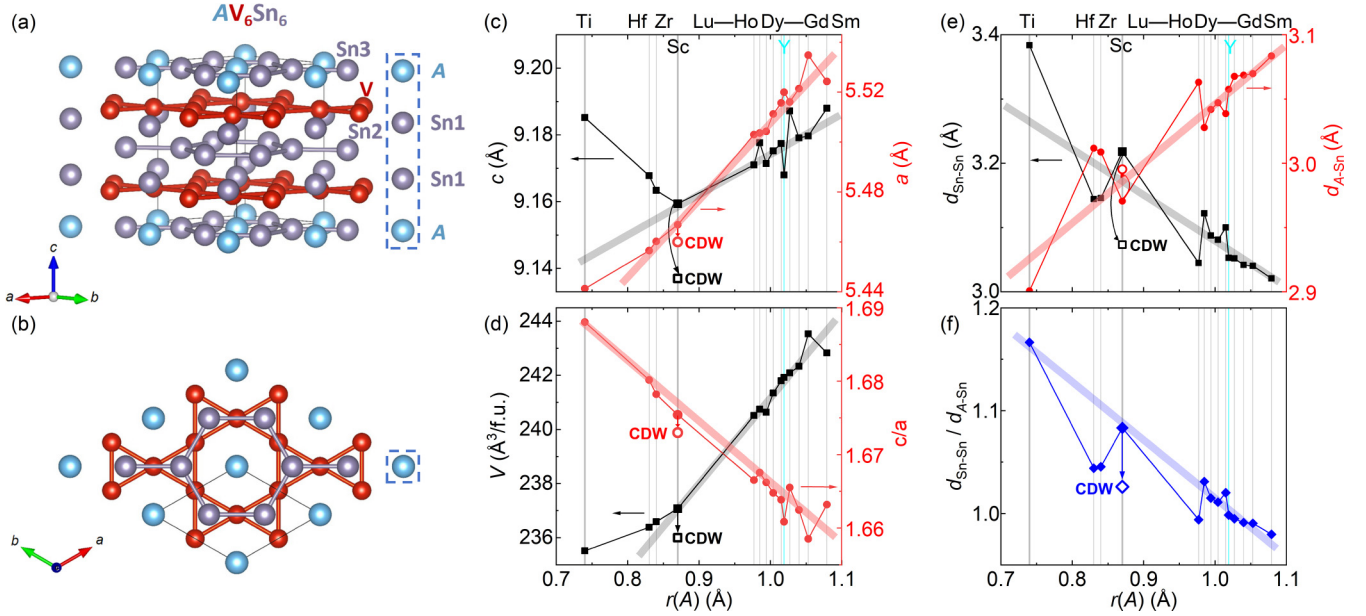


FIG. 1. (a) Perspective and (b) top views of the $HfFe_6Ge_6$ -type crystal structure of AV_6Sn_6 , with dashed lines indicating the A-Sn1-Sn1-A chain. (c)–(d) Evolution of the lattice parameters (c , a , V , and c/a) for all known AV_6Sn_6 compounds as a function of $r(A)$, the VIII-coordinated Shannon ion radius of the filler atom A [15]. (e)–(f) $r(A)$ dependence of the bond distances $d_{Sn1-Sn1}$ [(e), left axis], d_{A-Sn1} [(e), right axis], and $d_{Sn1-Sn1}/d_{A-Sn1}$ (f). Data for the charge density wave (CDW) phase of ScV_6Sn_6 are shown with open symbols. The lines in (c)–(f) are guides for eyes.

CDW transition was only observed in ScV_6Sn_6 , whereas no CDW signatures appear in TiV_6Sn_6 , ZrV_6Sn_6 , and HfV_6Sn_6 [14]. To obtain further insight into the rattling chain model, we systematically investigate the mechanism for the missing CDW transition in TiV_6Sn_6 .

Structural trend analysis of the AV_6Sn_6 family reveals that TiV_6Sn_6 satisfies all the structural criteria required by the rattling chain model. However, consistent with the previous report [14], no evidence of a CDW transition is observed in the resistivity, magnetization, and specific heat measurements. The absence of imaginary phonon modes further corroborates the absence of a CDW transition. The density functional theory (DFT) and COHP calculations show that TiV_6Sn_6 shares the general characteristics of AV_6Sn_6 , but possesses notable differences. Further analysis indicates that these differences, originating from Ti's relatively high electronegativity, are responsible for the absence of a CDW in TiV_6Sn_6 . The high electronegativity of Ti induces partially covalent interactions with neighboring atoms, which suppress the rattling behavior of Ti and eliminate CDW order. Our study demonstrates that the rattling chain model is not applicable to AM_6X_6 compounds containing filler atoms with a relatively high electronegativity. Accordingly, in addition to the ionic radius, electronegativity should be incorporated as a critical parameter to predict CDW in this model.

II. RESULTS AND DISCUSSION

A. Structural analysis

The crystal structure of the TiV_6Sn_6 crystals was determined by single-crystal XRD measurements, with the refined crystal structure shown in Figs. 1(a) and 1(b). The crystal crystallizes into the $HfFe_6Ge_6$ -type structure (space group

$P6/mmm$, No. 191), which comprises two kagome layers [$V_3(Sn1)_2$], one honeycomb layer [$(Sn2)_2$], and a triangular layer [$Ti(Sn3)_2$]. The chemical formula can be rewritten in structural form as $[Ti(Sn3)_2][V_3(Sn1)_2][(Sn2)_2][V_3(Sn1)_2]$. Structurally, TiV_6Sn_6 can be regarded as the Ti-stuffed $CoSn$ -type V_6Sn_6 [22]: Ti atoms occupy the hexagonal voids of the $Sn3$ honeycomb lattice and push the adjacent $Sn1$ atoms out of the V_3Sn1 layer, forming a Ti-Sn1-Sn1-Ti chain within the channels of the hexagonal voids in the kagome and honeycomb layers. According to the rattling chain model for AM_6X_6 compounds, if the filler atom A is small enough, the rattling of the A-X-X-A chain will drive a CDW phase transition [8,10]. Fortunately, Ti is the smallest atom that can form a stable structure among the known AV_6Sn_6 series ($A = Ti, Zr, Hf, Sc, Y, Sm$, and $Gd-Lu$) (Table I), motivating the choice of TiV_6Sn_6 for this study [10,14,23–25].

To assess the applicability of the rattling chain model to TiV_6Sn_6 , we analyze the structural trend of the AV_6Sn_6 ($A = Ti, Zr, Hf$, and rare earth $R = Sc, Y, Sm$, and $Gd-Lu$) family, with particular attention paid to the difference between TiV_6Sn_6 and ScV_6Sn_6 . As shown in Fig. 1(c), lattice parameters for AV_6Sn_6 on the left side of the phase diagram [$r \leq r(Zr)$] deviate from the linear trend on the right side [$r \geq r(Sc)$]. A similar deviation has also been observed in AF_6Ge_6 , which was attributed to the different chemical properties between the transition metals and rare-earth elements [11]. On the right side, the data can be well described by linear behavior, indicating that the crystal structure of rare-earth-based AV_6Sn_6 is primarily governed by the ionic radius $r(A)$. This phenomenon also indicates similar chemical properties within the rare-earth elements. However, when $r(A)$ decreases from Sc to Ti, c increases while a continuously decreases with a slightly slower rate. Consistently, Fig. 1(d) shows a slope

TABLE I. Lattice parameters of known AV_6Sn_6 , which are crystalline in $HfFe_6Ge_6$ -type structure with space group $P6/mmm$.

Compound	r_{ion} (Å)	a (Å)	c (Å)	V (Å ³)	c/a	d_{A-Sn} (Å)	d_{Sn-Sn} (Å)	d_{Sn-Sn}/d_{A-Sn}	T_N (K)	T_{CDW} (K)	Ref.
TiV ₆ Sn ₆	0.740	5.4413	9.1852	235.52	1.688	2.9007	3.3838	1.1665	—	—	This work
TiV ₆ Sn ₆	0.740	5.4452	9.1916	236.02	1.688	2.9017	3.3882	1.1677	—	—	[14]
HfV ₆ Sn ₆	0.830	5.4565	9.1678	236.39	1.680	3.0117	3.1444	1.0441	—	—	[14]
ZrV ₆ Sn ₆	0.840	5.4602	9.1634	236.59	1.678	3.0088	3.1458	1.0455	—	—	[14]
ScV ₆ Sn ₆	0.870	5.4669	9.1594	237.07	1.675	2.9706	3.2183	1.0834	—	92	[16]
LuV ₆ Sn ₆	0.977	5.5030	9.1710	240.52	1.667	3.0631	3.0447	0.9940	—	—	[17]
YbV ₆ Sn ₆	0.985	5.5036	9.1777	240.75	1.668	3.0278	3.1221	1.0311	0.4	—	[18]
TmV ₆ Sn ₆	0.994	5.5043	9.1714	240.64	1.666	3.0419	3.0876	1.0150	—	—	[19]
ErV ₆ Sn ₆	1.004	5.5113	9.1752	241.35	1.665	3.0471	3.0810	1.0111	—	—	[19]
HoV ₆ Sn ₆	1.015	5.5157	9.1774	241.80	1.664	3.0386	3.1001	1.0202	2.5	—	[19]
YV ₆ Sn ₆	1.019	5.5200	9.1680	241.93	1.661	3.0575	3.0529	0.9985	—	—	[20]
DyV ₆ Sn ₆	1.027	5.5161	9.1872	242.09	1.665	3.0676	3.0520	0.9949	3	—	[19]
TbV ₆ Sn ₆	1.040	5.5214	9.1791	242.34	1.662	3.0686	3.0420	0.9913	4.4	—	[19]
GdV ₆ Sn ₆	1.053	5.5348	9.1797	243.54	1.658	3.0697	3.0403	0.9904	5.2	—	[20]
SmV ₆ Sn ₆	1.079	5.5243	9.1880	242.83	1.663	3.0835	3.0210	0.9797	—	—	[21]

change in the volume V vs $r(A)$ curve below Sc. In contrast, the c/a ratio stays almost linear across the entire phase diagram. The deviation from the linear trend for $r(A) < r(Sc)$ implies that the structure of AV_6Sn_6 ($A = Ti, Zr, Hf$) depends on factors beyond the ionic radius, which should be different from those in the rare-earth elements. These structural trends are analogous to those in AFe_6Ge_6 , indicative of a similar underlying mechanism [11].

Based on the systematic structural trend analysis of the AV_6Sn_6 family above, we first revisit the fundamental structural criteria of the rattling chain model for predicting CDW order in kagome metals. The rattling chain model predicts CDW order in AM_6X_6 -type kagome metals based on two hierarchical core structural prerequisites: (i) a sufficiently small ionic radius of the A-site filler atom combined with a large host lattice that provides adequate void space for the rattling motion of the $A-X-X-A$ chain, and (ii) a large intrinsic $X-X$ bond length within the chain, which serves as the direct structural precursor for the CDW-driven $X-X$ dimerization. Our systematic crystallographic analysis demonstrates that TiV₆Sn₆ fully satisfies all the core structural criteria of the rattling chain model, which can be verified from two complementary dimensions: the evolution of global lattice parameters and the local bonding geometry of the rattling chain.

From the perspective of global lattice parameters in light of the rattling chain model, TiV₆Sn₆ exhibits structural features highly favorable for CDW formation. When the ionic radius of the A-site filler atom decreases from Sc to Ti, the c -axis lattice parameter increases and the unit cell volume V shows a distinct upturn [Figs. 1(c) and 1(d)]. This expanded c -axis channel, together with a unit cell volume comparable to that of ScV₆Sn₆, provides sufficient void space for the rattling motion of the Ti-Sn1-Sn1-Ti chain along the c direction, and is more conducive to satisfying the spatial requirements of the rattling chain model compared to the CDW-host compound ScV₆Sn₆.

Beyond the global lattice parameters, we further quantify the local bonding characteristics of the $A-Sn-Sn-A$ chain, which is structurally responsible for the CDW order. We plot d_{Sn-Sn} , d_{A-Sn} , and d_{Sn-Sn}/d_{A-Sn} against $r(A)$ in Figs. 1(e) and 1(f), with the data of CDW phase for ScV₆Sn₆ included for

direct comparison. In ScV₆Sn₆, the CDW transition induce -0.43% and -0.27% shrinkage in c and a , respectively; correspondingly, d_{Sn-Sn} decreases by -4.5% while d_{A-Sn} increases by 0.83% . This is consistent with the formation of Sn-Sn dimers along the c axis as the main character of CDW-induced structural distortion [16]. If the Sn-Sn dimerization is taken as the hallmark of the CDW-induced structural distortion in 166 compounds, then a relatively large d_{Sn-Sn} in the $A-Sn-Sn-A$ chain should be the criterion required by the rattling chain model, equivalent to the small ionic radius of filler atoms. Within the AV_6Sn_6 series, only TiV₆Sn₆ has a larger d_{Sn-Sn} than ScV₆Sn₆ [Fig. 1(e)], providing a plausible explanation for why the CDW transitions are absent in ZrV₆Sn₆ and HfV₆Sn₆, where the filler-ion size is also smaller than Sc [10]. From the systematic crystallographic analysis above, the key structural parameters of TiV₆Sn₆—including the c -axis lattice parameter, c/a ratio, d_{Sn-Sn} , d_{A-Sn} , and their ratio d_{Sn-Sn}/d_{A-Sn} —all fully satisfy the core criteria of the rattling chain model. Therefore, TiV₆Sn₆ satisfies all the structural requirements of the rattling chain model, and a CDW transition is expected.

B. Physical properties

Since the ionic radius depends sensitively on the valence, we first check the valence of Ti through the x-ray photoelectron spectroscopy (XPS) measurements. From Fig. 2(a), it can be seen that the Ti $2p_{3/2}$ binding energy matches well with that of TiO₂, indicating Ti⁴⁺ valence in TiV₆Sn₆. With an ionic radius of 0.606 Å [15], Ti⁴⁺ is the smallest among the filler atoms in AV_6Sn_6 compounds, and thus confirm the satisfaction of the key requirement of the rattling chain model [8].

To experimentally verify whether TiV₆Sn₆ undergoes a CDW transition as predicted by the structural criteria of the rattling chain model, we carried out electrical resistivity, magnetic susceptibility, and specific heat measurements on TiV₆Sn₆. These are standard and highly sensitive probes for identifying anomalies associated with phase transitions. Figure 2(b) presents the temperature dependence of the resistivity $\rho_{xx}(T)$, which shows metallic behavior. A pronounced

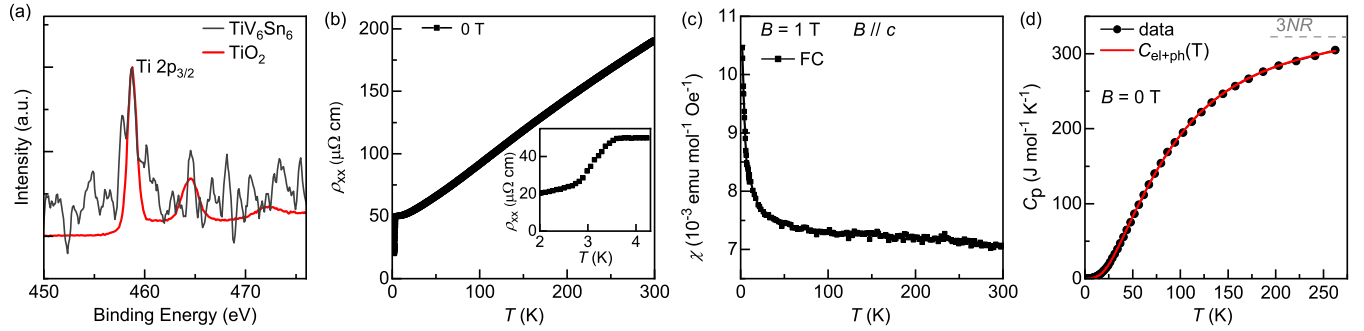


FIG. 2. (a) X-ray photoelectron spectroscopy of Ti $2p$ spectra for a TiV_6Sn_6 crystal and TiO_2 powder. (b) Temperature dependence of in-plane resistivity measured at $B = 0$ T for a TiV_6Sn_6 crystal. Inset shows the enlarged view of the low-temperature resistivity in the range of 2–4.5 K. (c) Temperature dependence of field-cooled (FC) magnetic susceptibilities measured with a $B = 1$ T field applied along the c axis of a TiV_6Sn_6 crystal. (d) Specific heat $C_p(T)$ ($B = 0$ T) as a function of temperature for a TiV_6Sn_6 crystal. The red line is a fit to the data using the Debye-Einstein model. The horizontal dashed line represents the Dulong-Petit limit.

drop appears at 3.6 K, arising from the superconducting transition of residual Sn flux on the crystal surface [24]. The nearly linear $\rho_{xx}(T)$ in TiV_6Sn_6 resembles that of non-CDW RV_6Sn_6 compounds ($A = \text{Y, Gd-Lu}$) [14,23,24], but contrasts with the sublinear $\rho_{xx}(T)$ observed in ScV_6Sn_6 and AV_3Sb_5 ($A = \text{K, Rb, and Cs}$), which has been reported as a universal feature of vanadium kagome materials exhibiting charge density waves [26]. As shown in Fig. 2(c), the magnetic susceptibility $\chi(T)$ of TiV_6Sn_6 follows a general behavior of the nonmagnetic AV_6Sn_6 series ($A = \text{Ti, Zr, Hf, Lu, Y}$) [14,24], displaying weak Pauli paramagnetism at elevated temperatures and a small Curie-Weiss upturn at low temperatures. In addition, Fig. 2(d) shows that the specific heat $C_p(T)$ from 2 to 300 K can be well described by the Debye-Einstein model [27], with no detectable anomaly that would indicate a phase transition. Taken together, the resistivity, magnetization, and specific heat results reveal no evidence for a CDW transition in TiV_6Sn_6 , in agreement with previous work [14].

C. Phonon spectrum

Both Fermi surface nesting (FSN)- and electron-phonon coupling (EPC)-driven CDWs exhibit phonon softening at T_{CDW} , making the imaginary phonon mode an important signature of CDW instability [28]. To get further insight into the CDW transition in TiV_6Sn_6 , we performed phonon calculations on the pristine and strained structures, with the results shown in Fig. 3. The phonon characteristics of pristine TiV_6Sn_6 can be elucidated by comparison with those of ScV_6Sn_6 . As shown in Fig. 3(c), the phonon spectrum of TiV_6Sn_6 closely resembles that of ScV_6Sn_6 , particularly for the V-, Sn2-, and Sn3-derived branches. The primary differences lie in the Sc/Ti-derived phonon bands at high frequencies and Sn1-derived phonon bands at low frequencies. As indicated by the shaded regions in Fig. 3(c), the Sc-derived phonon bands around 5.3 and 7.2 THz are remarkably flat across the Brillouin zone, signifying localized Sc vibrations arising from weak interatomic interactions. Conversely, the Ti-derived bands are more dispersive, suggesting stronger interatomic bonding with adjacent atoms. Furthermore, ScV_6Sn_6 displays flat imaginary modes across the entire $k_z = \pi$ plane (i.e., the A - L - H plane), which are

dominated by the out-of-plane vibrations of Sc and Sn1 atoms [30,31]. It is the softening of these flat phonon bands in the $k_z = \pi$ plane that derives multiple charge instabilities in ScV_6Sn_6 [30–33]. Similarly, TiV_6Sn_6 also features its softest phonon bands within the $k_z = \pi$ plane, with the minimum located at the H point. However, in contrast to ScV_6Sn_6 , all the phonon modes in TiV_6Sn_6 remain positive, indicating the absence of lattice instabilities.

In fact, the rare-earth-based RV_6Sn_6 ($R = \text{Y, Gd, Tb, Dy, Ho, Er, Tm, and Lu}$) exhibits a phonon spectrum similar to that of TiV_6Sn_6 , where the lowest phonon band lies in the $k_z = \pi$ plane and remains fully positive (see Fig. S2(b) in the Supplemental Material of Ref. [34]). Consistent with the rattling chain model, the lowest phonon branch in RV_6Sn_6 progressively softens as the ionic radius of R decreases, reaching a minimum in LuV_6Sn_6 due to Lu^{3+} having the smallest ionic radius among these rare-earth atoms. Although the imaginary phonon mode cannot be obtained by further reducing the ionic size of the filler atom, it can be induced by both in-plane compression and out-of-plane extension of the lattice [34], further validating the rattling chain model and confirming its applicability to rare-earth stuffed RV_6Sn_6 compounds. However, as shown in Fig. 3, applying uniaxial strain along the c axis, either compressive (-2% , -5%) or tensile ($+2\%$, $+5\%$), does not produce any imaginary phonon modes in TiV_6Sn_6 . Instead, the lowest phonon branch along the $L-H$ line gradually hardens under both compressive and tensile strains. Although pristine TiV_6Sn_6 shares a similar phonon spectrum with RV_6Sn_6 , its response to the uniaxial strain deviates markedly from that of the rare-earth analogues. This divergence further corroborates the absence of a CDW transition in physical property measurements.

D. Band structure

In TiFe_6Ge_6 , the band structure differs significantly from other AF_6Ge_6 ($A = \text{Li, rare earth}$): instead of a rigid band shift induced by carrier doping, the density of states shifts away from the E_F , accompanied by the appearance of a hole pocket with Ti orbital character [11]. Such differences were regarded as the consequence of the covalent bonding character of Ti and play a key role in the absence of CDW in

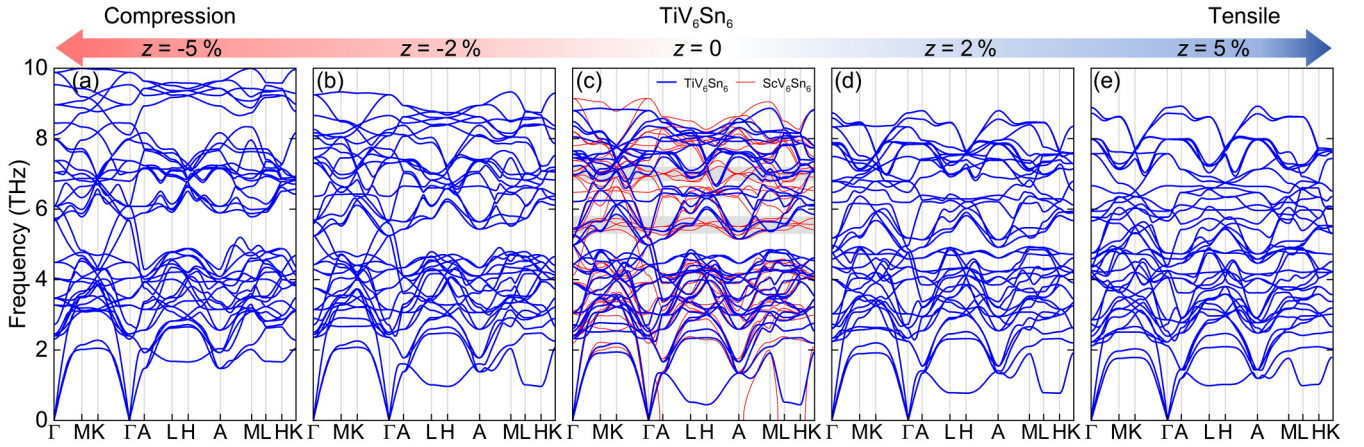


FIG. 3. Phonon spectra of TiV_6Sn_6 under out-of-plane (c -axis) uniaxial strains. (a) and (b) show compressive strains of $z = -5\%$ and $z = -2\%$, respectively; (c) corresponds to the pristine structure ($z = 0$); (d) and (e) correspond to tensile strains of $z = +2\%$ and $z = +5\%$, respectively. For comparison, (c) also includes phonon spectrum of pristine ScV_6Sn_6 , where the gray shading indicates the flat Sc-derived phonon modes. Further details and the corresponding lattice parameters are provided in the Supplemental Material [29]. Unlike ScV_6Sn_6 , TiV_6Sn_6 shows no imaginary modes, and the phonon branches along $L-H$ harden under both compressive and tensile strains.

TiFe_6Ge_6 . We perform the DFT calculation on TiV_6Sn_6 , with the results shown in Figs. 4(a)–4(d). In marked contrast to that of TiFe_6Ge_6 , the band structure of TiV_6Sn_6 shares the general behavior of RV_6Sn_6 , ZrV_6Sn_6 , and HfV_6Sn_6 , characterized by typical kagome band features, i.e., van Hove singularities (VHSs) at M/L points, Dirac points at K/H points, a nodal

ring (NR) along $K-\Gamma$ line, and a flat band at approximately 0.2 eV [14,20,34–37]. As revealed by the atom-resolved band structure in Fig. 4 and density of states in Fig. S7 in the Supplemental Material [29], the bands around E_F for TiV_6Sn_6 are dominated by V-derived orbitals with a minor contribution from Ti and Sn1, whereas the contributions from Sn2 and Sn3

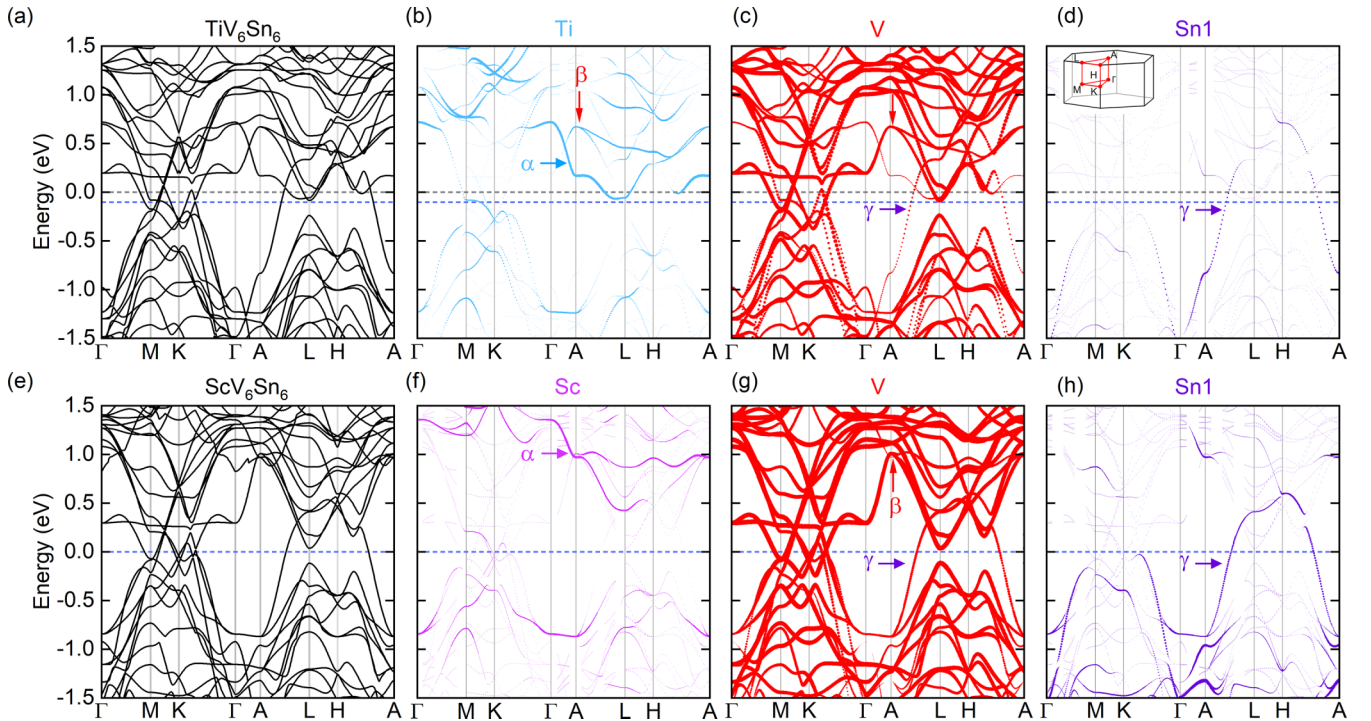


FIG. 4. (a) Band structure for TiV_6Sn_6 and (b) atom-resolved band structures for Ti, (c) V, and (d) Sn1 atoms, respectively. The gray and blue horizontal dashed lines denote the Fermi level (E_F) of TiV_6Sn_6 and ScV_6Sn_6 , respectively. The inset of (d) shows the Brillouin zone with high symmetry points labeled. The corresponding bands for ScV_6Sn_6 are shown in (e)–(h) for direct comparison. The arrows in (b)–(d) and (f)–(h) highlight bands exhibiting significant differences between the two compounds. Atom-resolved band structures for Sn2 and Sn3 atoms are provided in Fig. S9 of the Supplemental Material [29], and orbital-resolved band structures for each atom are presented in Figs. S10–S14 in Supplemental Material [29].

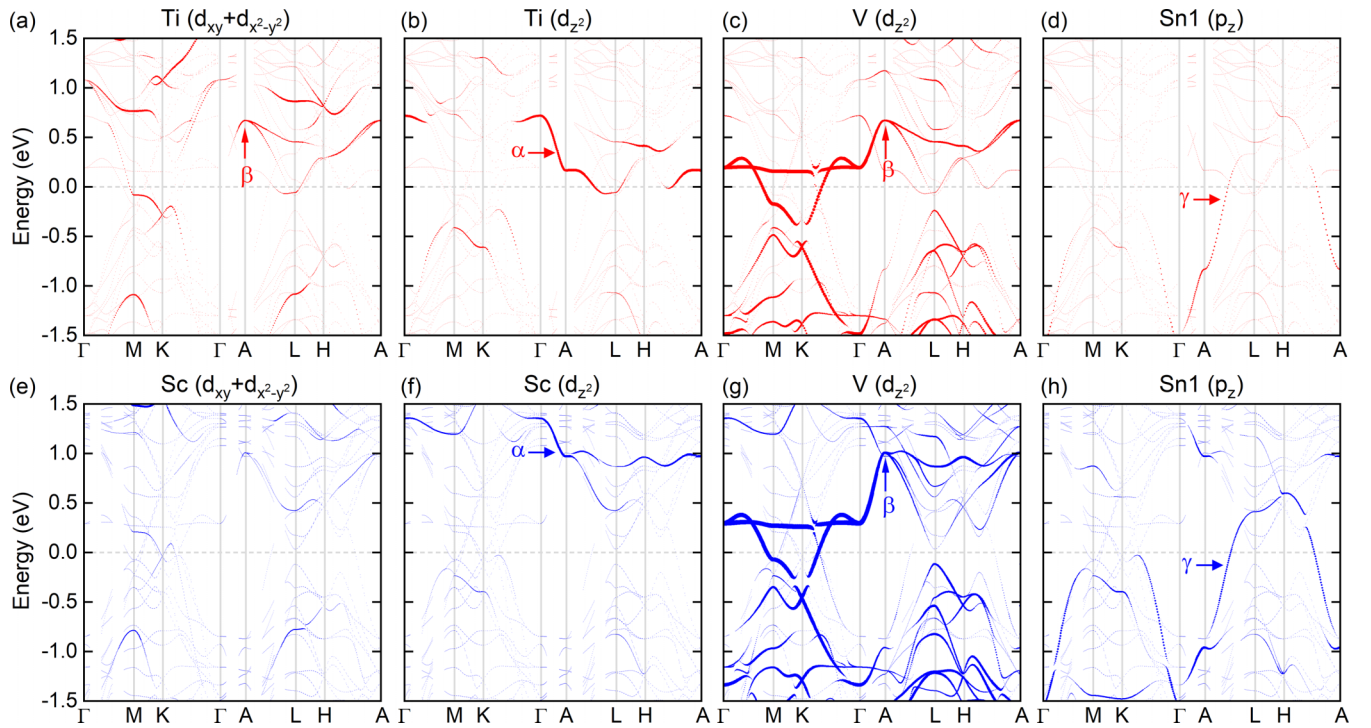


FIG. 5. Selected orbital-resolved band structures of (a)–(d) TiV_6Sn_6 and (e)–(h) ScV_6Sn_6 , showing pronounced difference between these two compounds. A complete orbital-by-orbital comparison is provided in the Supplemental Material [29].

are negligible (Figs. S7 and S9 in the Supplemental Material [29]). The kagome bands originate mainly from the V-derived orbitals and feature: VHSs at $E = 0.27$ and -0.18 eV (with $d_{yz} + d_{xz}$, $d_{xy} + d_{x^2-y^2}$, and d_{z^2} characters); Dirac points at $E = 0.6$ and 0.5 eV ($d_{xy} + d_{x^2-y^2}$ and $d_{yz} + d_{xz}$); a nodal ring at $E = 0.06$ eV ($d_{xy} + d_{x^2-y^2}$ and $d_{yz} + d_{xz}$); and a flat band at $E \sim 0.2$ eV, primarily derived from d_{z^2} states (see Fig. S11 in Supplemental Material [29]). In addition to these V-derived kagome bands, the Ti d_{z^2} and Sn1 p_z orbitals also cross the E_F within the $k_z = \pi$ plane, as marked by α and γ in Figs. 4(b) and 4(d).

The clue for the absence of a CDW transition in TiV_6Sn_6 could be inferred from the comparison of the band structure with ScV_6Sn_6 (Figs. 4 and 5). Although Ti does not alter the band structure as drastically as in TiFe_6Ge_6 , notable differences relative to $R\text{V}_6\text{Sn}_6$ ($R = \text{Sc}, \text{Y}$, and rare earth) can still be identified (Figs. 4 and 5 and Figs. S8–S15 in Supplemental Material [29]), where the orbitals that show pronounced differences are plotted in Fig. 5. First, the E_F is increased by ~ 0.1 eV, which is consistent with the Hall measurements (Fig. S3 in Supplemental Material [29]) and can be attributed to an extra electron donated by Ti^{4+} . Note that our calculated E_F is slightly higher than the previous report [14], approaching the Dirac cone/nodal ring along the M - K and K - Γ lines, which may be responsible for the different MR behavior in our crystals (Fig. S2(a) in Supplemental Material [29]). Second, the α band, dominated by Ti d_{z^2} orbital character, shifts downward, crosses the E_F , and forms a hole pocket [Fig. 5(b)]. This behavior resembles that in TiFe_6Ge_6 [11, 14], but contrast with ScV_6Sn_6 , where no Sc-derived band cross E_F [34]. Third, the β band, dominated by V d_{z^2} orbital, also shows a clearly downward shift [Fig. 5(c)]. Fourth, the γ band, dominated by

Sn p_z orbital, critical for the CDW instability in ScV_6Sn_6 , shifts a little upward, accompanied by significant weight loss [Fig. 5(d)].

E. Chemical bonding

During the study of TiFe_6Ge_6 , we found that the absence of CDW can be attributed to the bonding characteristics of Ti [11]. Among the filler atoms in $A\text{Fe}_6\text{Ge}_6$, Ti differs significantly from that of Li and the rare-earth elements: Ti forms strong covalent bonds with adjacent atoms, and its electrons are primarily localized in Ti-Ge1b bonds rather than delocalized throughout the crystal [11]. The formation of strong covalent bonding within the Ti-Ge1b-Ge1b-Ti chain, specifically the Ti-Ge1b and Ge1b-Ge1b bonds, prevents the chain from rattling, resulting in the absence of a CDW transition in TiFe_6Ge_6 . Phonon spectrum analysis in TiV_6Sn_6 also revealed that Ti behaves differently from Sc and other rare-earth elements, implying a similar mechanism for the absence of CDW in both compounds.

To investigate the bonding in TiV_6Sn_6 , we performed COHP analysis using the LOBSTER package. The COHP curves for representative interatomic bonds in TiV_6Sn_6 (black), ScV_6Sn_6 in the normal state (red lines), and ScV_6Sn_6 in the CDW state (blue) are shown in Fig. 6. From Figs. 6(a)–6(f), it can be seen that the black curves are shifted downward by approximately 0.1 eV relative to the red curves, consistent with the band structure in Fig. 4. This is a characteristic of electron doping: Ti donates more electrons than Sc, raising E_F , which is equivalent to a rigid downward shift of the COHP curves. Beyond this rigid shift, subtle differences are evident, particularly for Ti-V, Ti-Sn3, Ti-Sn1, and

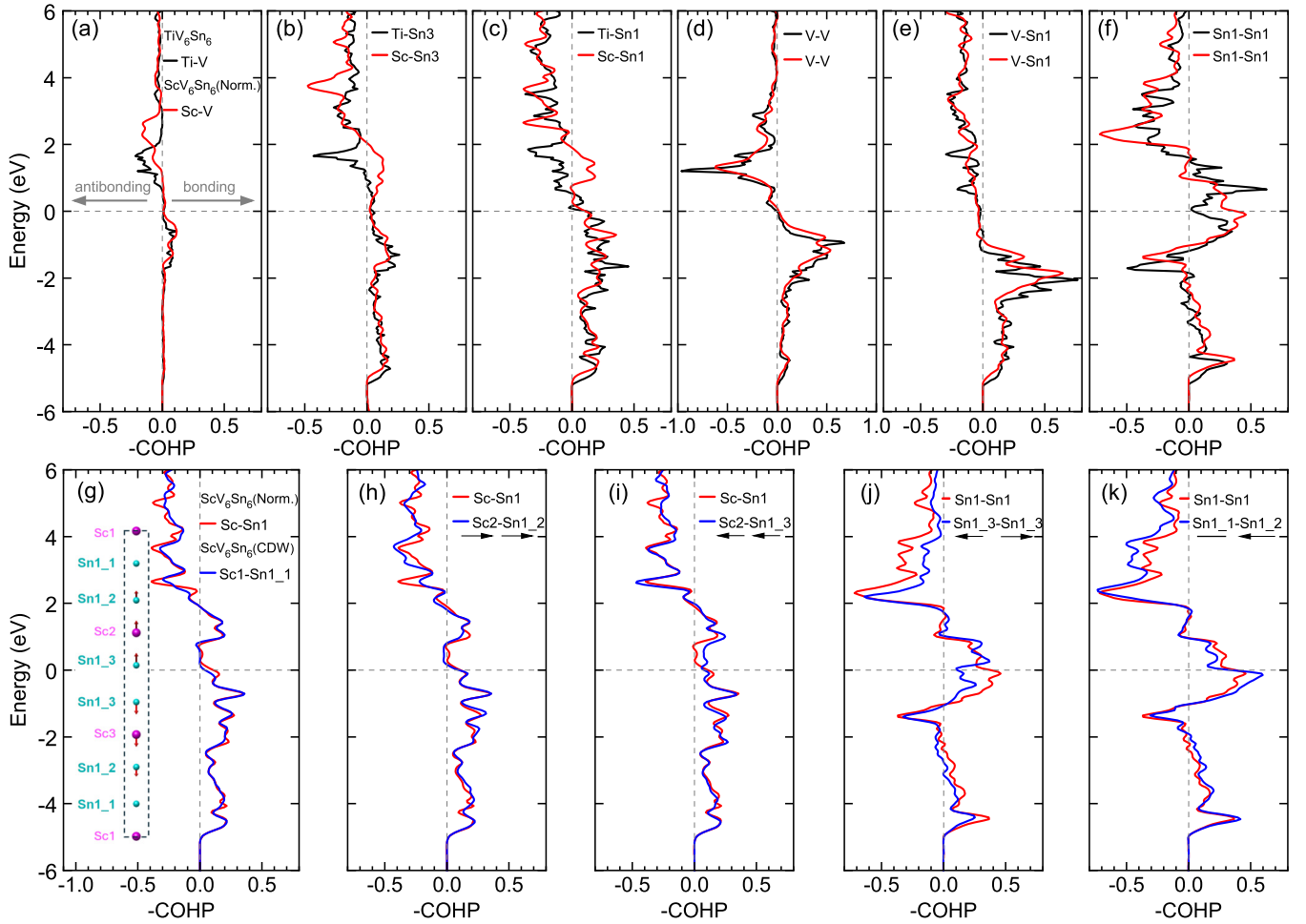


FIG. 6. Crystal orbital Hamilton population (COHP) analysis of the chemical bonding in TiV_6Sn_6 and ScV_6Sn_6 . Black, red, and blue lines represent the data for TiV_6Sn_6 , normal-state ScV_6Sn_6 , and CDW-state ScV_6Sn_6 , respectively. (a)–(f) COHP curves for representative interatomic bonds: (a) Ti-V and Sc-V, (b) Ti-Sn3 and Sc-Sn3, (c) Ti-Sn1 and Sc-Sn1, (d) V-V, (e) V-Sn1, and (f) Sn1-Sn1. The crystallographic atomic labels can be found in Fig. 1(a). Comparison of COHP curves between normal-state (red lines) and CDW-state (blue lines) of ScV_6Sn_6 for (g) Sc-Sn1 and Sc1-Sn1_1, (h) Sc-Sn1 and Sc2-Sn1_2, (i) Sc-Sn1 and Sc2-Sn1_3, (j) Sn1-Sn1 and Sn1_3-Sn1_3, and (k) Sn1-Sn1 and Sn1_1-Sn1_2 bonds. The CDW-induced atomic displacement within the Sc-Sn1-Sn1-Sc chain and corresponding atomic labels are shown in the inset of (g).

Sn1-Sn1 bonds. In TiV_6Sn_6 , E_F lies at the crossover between bonding and antibonding states for Ti-V, Ti-Sn3, and Ti-Sn1 bonds, rather than at the minimum of the bonding states as in ScV_6Sn_6 , indicating covalent bonding interaction. Based on the peak magnitude and integrated crystal orbital Hamilton population (ICOHP) values (Fig. 6 and Table II), the strength of the covalent interaction gradually increases in the order $\text{Ti-V} < \text{Ti-Sn3} < \text{Ti-Sn1}$, consistent with the bond length. Sc-V, Sc-Sn3, and Sc-Sn1 bonds follow a similar trend, but with a weaker and more ionic character, consistent with the electronegativity difference (Sc: 1.36, Sn: 1.96). The V-V COHP profiles are very similar between the two compounds. Antibonding peaks above E_F are enhanced for V-Sn1 in TiV_6Sn_6 . The most pronounced difference lies in the Sn1-Sn1 bonds: its bonding strength in TiV_6Sn_6 is significantly weaker than that in the normal state of ScV_6Sn_6 , close to the elongated Sn1-Sn1 bonds in the CDW phase of ScV_6Sn_6 [blue curve in Fig. 6(j)].

From the above analysis, it can be concluded that Ti exhibits mixed ionic and covalent bonding in TiV_6Sn_6 : it

partially donates electrons to the lattice and partially forms covalent bonds with adjacent atoms. This differs from the nearly completely covalent bonding in TiFe_6Ge_6 [11]. Unlike the stiff Ti-Ge1b-Ge1b-Ti chain in TiFe_6Ge_6 with strong Ti-Ge1b and Ge1b-Ge1b bonding, the Ti-Sn1-Sn1-Ti chain in TiV_6Sn_6 features a relatively strongly bonded Ti-Sn1 and weakly bonded Sn1-Sn1. In principle, this bonding character is consistent with the rattling chain model, where Sn1-Sc-Sn1 units move upward/downward as a whole in ScV_6Sn_6 to form the Sn1-Sn1 dimers arranged in a $3 \times 3 \times 3$ superstructure [16]. From this scenario, the weakened Sn1-Sn1 bond disfavors the dimerization required for CDW formation. However, because the bonding strength of Sn1-Sn1 is tunable by uniaxial strain and both the compressive and tensile strains harden the phonon modes (Fig. 3), the elongated Sn1-Sn1 bond distance might not be the main reason for the absence of the CDW transition. The primary reason should be Ti's covalent interaction with its neighbors. Although much weaker than that in TiFe_6Ge_6 , this interaction is stronger than that in ScV_6Sn_6 and sufficient to prevent rattling

TABLE II. ICOHP values and bond lengths of key interatomic bonds in TiV_6Sn_6 , normal-state ScV_6Sn_6 , and CDW-state ScV_6Sn_6 .

Material	Bond	Bond length (Å)	ICOHP (eV)
TiV_6Sn_6	Ti-V	3.5451	0.18856
	Ti-Sn3	3.1415	0.80255
	Ti-Sn1	2.9007	1.47337
	V-V	2.7207	0.97677
	V-Sn1	2.7922	1.44878
	Sn1-Sn1	3.3838	0.58005
ScV_6Sn_6 (normal)	Sc-V	3.5514	0.21643
	Sc-Sn3	3.1563	0.84026
	Sc-Sn1	2.9706	1.37304
	V-V	2.7335	0.95660
	V-Sn1	2.8225	1.37668
	Sn1-Sn1	3.2183	0.95208
ScV_6Sn_6 (CDW)	Sc1-Sn1_1	2.9954	1.29536
	Sc2-Sn1_2	2.9238	1.46779
	Sc2-Sn1_3	2.9488	1.34995
	Sn1_3-Sn1_3	3.5296	0.37895
	Sn1_1-Sn1_2	3.0735	1.38053

of the Ti-Sn1-Sn1-Ti chain, thereby suppressing the CDW transition.

F. Discussion

Taken together with the results of the phonon spectrum, electronic structure, and COHP data, we can conclude that the covalent bonding character of Ti is likely responsible for the absence of CDW in TiV_6Sn_6 . This interpretation is consistent with the difference between Ti and rare earth in structure trend, phonon spectra, and band structure. Due to the similar bonding character, rare-earth-based RV_6Sn_6 ($R = \text{Sc}, \text{Y}, \text{Sm}, \text{Gd-Lu}$) share a common electronic structure, for which the rattling chain model applies, in stark contrast to the Ti-based case. The distinction in the bonding character can be attributed to the difference in electronegativity, where the electronegativity of Ti (1.54) is higher than Sc, Y, and the rare-earth elements (< 1.36). Due to its higher electronegativity, Ti more readily forms covalent bonds with neighboring atoms, which inhibits the rattling motion of Ti and consequently suppresses the CDW transition. This likely accounts for the observation of CDW in strained RV_6Sn_6 but not in TiV_6Sn_6 .

Lattice vibrations in real space can equivalently be described by the phonon spectrum in reciprocal space. In the rattling chain model, the CDW formation in AM_6X_6 compounds is attributed to the out-of-plane motion of an $A\text{-X-X-A}$ chain residing in the hexagonal voids formed by the kagome and honeycomb layers [8,10]. From the perspective of the phonon spectrum, the motion of the $A\text{-X-X-A}$ chain is manifested as the flat phonon bands along the $A\text{-L-H-A}$ path ($k_z = \pi$ plane) [30,31]. Softening of these flat phonon bands drives abundant competing charge density waves (CDWs); specifically, imaginary phonon frequencies at different Brillouin-zone points correspond to distinct structural modulations, i.e., different patterns of Sn1-Sn1 dimers [31,32]. The influence of the filler ionic radius is reflected in the magnitude of this flat phonon branch: it is imaginary

in ScV_6Sn_6 but becomes positive for RV_6Sn_6 , with its value increasing systematically with the ionic radius of R [34]. In TiV_6Sn_6 , the more covalent character of Ti results in more dispersive, Ti-dominated phonon branches and a qualitatively different tensile response of the flat phonon mode (Fig. 3). Consequently, in TiV_6Sn_6 , the hardening of the lowest phonon branch under tensile strain is likely due to the reduction of the in-plane lattice constant a , which strengthens the bonding between Ti and its neighboring atoms. Under compressive strain, by contrast, hardening is instead linked to a contraction of the out-of-plane lattice parameter c , which reduces the available space for rattling [8]. Therefore, the lowest phonon band hardens under both compressive and tensile strain, indicating that no CDW transition occurs.

The difference in the band structure between TiV_6Sn_6 and ScV_6Sn_6 can be understood as a consequence of the unique bonding character of Ti. In TiV_6Sn_6 , Ti exhibits mixed ionic and covalent bonding: the ionic component donates electrons to the lattice, raising E_F by ~ 0.1 eV, while the covalent component localizes electrons, leading to the downshift of the α and β bands. Both the α and β bands show Ti-V orbital hybridization character, specifically Ti d_{z^2} with V $d_{xy} + d_{x^2-y^2}$ for α band, V d_{z^2} with Ti $d_{xy} + d_{x^2-y^2}$ for β band (see Figs. S10 and S11 in the Supplemental Material [29]). The enhanced Ti-V bonding strength drives the downshift of α and β bands. The weight loss of the γ band can be attributed to the strong Ti-Sn1 covalent interaction, as Ti withdraws more electron density from Sn1 than Sc does. This strong covalency also acts as a negative factor for the formation of Sn1-Sn1 dimers. Compared to TiFe_6Ge_6 , the covalent interactions involving Ti are relatively weak, which does not alter the band structure severely, such as opening a gap along the $k_z = 0$ plane. However, these bonding interactions are stronger than those involving rare-earth elements and are sufficient to prevent Ti atoms, and consequently the Ti-Sn1-Sn1-Ti chain, from rattling, thereby suppressing the CDW transition.

In this work, the phonon spectrum and electronic structure of TiV_6Sn_6 are predicted using DFT calculations. We would like to point out that, although direct experimental evidence is currently lacking, the reliability of our calculations is strongly supported by their correctness in the sister compound ScV_6Sn_6 . Both materials share the same nonmagnetic crystal structure, and the DFT framework used in this work has been extensively validated for ScV_6Sn_6 through various experimental techniques, including inelastic x-ray [30,32], synchrotron x-ray [9], Raman spectroscopy [38], strain effect measurements [39], and angle-resolved photoemission spectroscopy (ARPES) measurements [30,40–43]. Furthermore, the correctness of our calculations is corroborated by comparisons with previous results [14] and with the sister compounds ScV_6Sn_6 and TiFe_6Ge_6 [11,31]. Nevertheless, direct experimental validation of our predictions remains highly desirable. Specifically, future inelastic x-ray/neutron scattering and Raman spectroscopy measurements are needed to probe the phonon spectrum, while ARPES and scanning tunneling microscopy (STM) would be essential for mapping the electronic structure.

Single-crystal XRD refinement indicates full occupancy of the Ti and V Wyckoff sites in our TiV_6Sn_6 crystals, whereas

energy-dispersive x-ray spectroscopy gives a Ti:V:Sn ratio of 1.11:5.73:6.00, suggesting Ti-V disorder. This discrepancy likely stems from the similar atomic numbers of Ti and V, which makes them hard to differentiate using XRD. As noted by Ortiz *et al.* [10], this type of disorder may suppress the anticipated CDW order in real samples, offering a possible explanation for why a CDW is not observed in TiV_6Sn_6 [10,14]. It is worth emphasizing that our DFT calculations and bonding analyses were performed on an ideal, fully ordered crystal structure with no Ti-V disorder. Even under this ideal assumption, the computed phonon spectra and electronic band structures consistently indicate the absence of a CDW in TiV_6Sn_6 . Thus, the lack of CDW order in TiV_6Sn_6 appears to be intrinsic, primarily tied to differences between Ti and rare-earth elements—most notably Ti's higher electronegativity, as discussed above.

III. CONCLUSION

In conclusion, we systematically investigated the origin of the absence of the CDW transition in TiV_6Sn_6 , which should be a CDW material according to the rattling chain model. Although rare-earth-based RV_6Sn_6 compounds share highly similar phonon and electronic structures, TiV_6Sn_6 shows subtle but identifiable differences. No imaginary phonon modes appear under either compressive or tensile strain. COHP and band structure analyses reveal that Ti exhibits a mixed ionic and covalent bonding; its covalent interactions with neighboring atoms inhibit rattling, thereby suppressing the CDW transition. The observed differences in the phonon spectra, electronic structure, and bonding character between TiV_6Sn_6 and RV_6Sn_6 stem from the differences in electronegativity. Specifically, Ti's higher electronegativity promotes covalent bonding. Our results indicate that, beyond ionic radius, the electronegativity of the filler atom should be taken into account in the rattling chain model.

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DATA AVAILABILITY

There are no publicly available research data or software supporting this paper. Requests for further information or data should be sent to the authors.

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