# Spin-orbit driven Peierls transition and possible exotic superconductivity in $CsW_2O_6$

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We study *ab initio* a pyrochlore compound, $CsW_2O_6$, which exhibits a yet unexplained metal-insulator transition. We find that (1) the reported low-$T$ structure is likely inaccurate and the correct structure has a twice larger cell; (2) the insulating phase is not of a Mott or dimer-singlet nature, but a rare example of a 3D Peierls transition, with a simultaneous condensation of three density waves; (3) spin-orbit interaction plays a crucial role, forming well-nested bands. The high-$T$ (HT) phase, if stabilized, could harbor a unique $e_g + ie_g$ superconducting state that breaks the time reversal symmetry, but is not chiral. This state was predicted in 1999, but never observed. We speculate about possible ways to stabilize the HT phase while keeping the conditions for superconductivity.

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*Introduction.* Insulating transition metal compounds with partially filled $d$ shell most often turn out to be locally magnetic (either forming a long-range magnetic order or remaining paramagnetic). There are some exceptions to this rule when, for instance, a transition metal ion is in the low-spin configuration due to a strong crystal-field splitting[1]. Alternatively, a Haldane state may appear in low-dimensional materials with integer spins, as e.g. in $Tl_2Ru_2O_7$[2]. Yet another possibility is formation of spin-singlet molecular clusters, such as dimers and timers (as it happens in $VO_2$[1], $Li_2RuO_3$ [3–6] or $Ba_4Ru_3O_{10}$ [7, 8]) or even more complex objects (heptamers in $AlV_2O_4$[9] or octamers in $CuIr_2S_4$[10]). However, in order to get a singlet ($S = 0$) ground state one needs an even number of electrons (doubly) occupying lowest energy levels in such clusters, as it occurs in $Li_2RuO_3$ or $AlV_2O_4$. In this sense a recent discovery of zero magnetic susceptibility in the insulating $\beta-$pyrochlore $CsW_2O_6$, with average occupancy $1/2$ electron per site, looks very unusual[11].

This compound undergoes a metal-insulator transition at 210 K with a Pauli-like magnetic susceptibility for $T > 210$ K, while at lower temperatures, in an insulating phase, it is fully nonmagnetic [11]. The high temperature (HT) phase is cubic (space group $Fd3m$)[12]. A complicated structure was proposed for the low temperature (LT) phase, with a doubled unit cell (compared to the FCC Bravais lattice of two formula units), with a disproportionation into two types of W and three types of W-W bonds. The short bonds form 1D zigzag chains[11]. At the same time, the average W-O distance (the valence bond sum) is nearly the same for both W, indicating absence of a charge order. Obviously, uniform 1D chains with noninteger number of electrons per site cannot form a simple band insulator.

The insulating and nonmagnetic nature of the low-temperature phase of $CsW_2O_6$, given the absence of charge disproportionation, no di- or tetramer formation, and $1/2$ electron per metal site, remains mysterious. Most usual suspects for explaining such transitions patently fail in $CsW_2O_6$. Indeed,

(i) Strong spin-orbit coupling (SOC), typical for $5d$ metals such as W, in principle may stabilize a nonmagnetic state with the orbital moment antiparallel to spin and the total moment $J = 0$. However, while this may be the case for $d^4$ configuration[1, 13], it is not possible for the $d^{1/2}$ occupancy. Besides, this model cannot explain the insulating behavior.

(ii) Correlation effects such as a Mott-Hubbard transition with possible formation of spin-singlets below 210 K would result in formation of local spin moments, manifestly absent at any temperature.

(iii) In principle, exotic electron-phonon coupling could stabilize bipolarons, whereupon every fourth W would have a nonmagnetic $d^2$ configurations, and all others the nonmagnetic $d^0$. However, that would generate a considerable O breathing distortion around the $d^2$ atom, which would be hardly possible to miss in the experiment. Besides, that would have to work against the Hubbard $U$, which, while small in W, would still amount to at least 1 eV.

We are left with the only possible scenario: the metal-insulator transition here is of the Peierls type, and the low-T state is a band insulator. The reported low-T structure [11] does show symmetry lowering: along the W-W nearest neighbor directions the bonds alternate as short-short-long-long, reminiscent of the proposition of Mizokawa and Khomskii[14], who suggested that, in analogy with $MgTi_2O_4$, in $CuIr_2S_4$ $1/2$ hole per metal can form a quasi-1D band along the Ir-Ir bonds, resulting in a Peierls transition with tetramerization, e.g., $Ir^{3+}/Ir^{3+}/Ir^{4+}/Ir^{4+}/...$ However, the experimentally suggested structure exhibits a different pattern, $W^{5.5+x}/W^{5.5-x}/W^{5.5+x}/W^{5.5-x}/...$, and experi-

ment does not show any charge disproportionation. That is to say, the structure proposed in Ref. [11] still leaves uniform quasi-1D zigzag chains, running along the crystallographic $b$ direction, which generate very metallic bands that cannot open a gap even if the DFT bands are slightly off (see discussion below and the corresponding band structure in Supplemental Materials (SM)). This suggests that the real crystal structure for the low-T phase may have lower symmetry than that proposed in Ref. [11]. We will argue below that the transition in question is actually a 3D Peierls transition, and that the true LT structure encompasses four, not two cubic cells. 3D Peierls transitions are extremely rare, but not impossible (for instance, the nearest-neighbor $sp\sigma$ tight-binding model on the perovskite lattice at some filling exhibits a perfect 3D nesting at $\mathbf{k} = [\frac{\pi}{a}, \frac{\pi}{a}, \frac{\pi}{a}]$ [15]).

We will present below accurate DFT calculations of the electronic structure of $CsW_2O_6$, and will show that upon including the spin-orbit interaction (which appears essential for explaining the phase transition) it exhibits a surprisingly simple Fermi surface (FS) with strong nesting for the three equivalent wave vectors $\mathbf{Q}_1 = [\frac{2\pi}{a}, 0, 0]$, $\mathbf{Q}_2 = [0, \frac{2\pi}{a}, 0]$, $\mathbf{Q}_3 = [0, 0, \frac{2\pi}{a}]$. This is conducive to simultaneous condensation of the three corresponding charge density waves (CDWs). Importantly, such condensation corresponds to a four-, not eightfold supercell, as one may think. The phonon spectra indicates instability exactly at these $\mathbf{Q}_1, \mathbf{Q}_2$, and $\mathbf{Q}_3$ points and optimizing crystal lattice starting from a structure inspired by these phonon modes we obtained a lower symmetry structure that opens a band gap. This structure is much lower in energy than the published structure and yields a nonmagnetic ground state, which agrees completely with experiment.

Finally, we will discuss an intriguing implication of stabilizing the HT structure at low temperature. We will argue that such a system could harbor a highly unusual, and so far never observed, albeit theoretically predicted, superconducting state.

*Computational results.* The DFT calculations were performed using the full potential Linearized Augmented Plane Wave (LAPW) method (as implemented in the Wien2k package[16]) with the Perdew-Burke-Ernzerhof (PBE) exchange-correlation potential[17]. The noninteracting susceptibility was computed on a fine mesh of 36000 $\mathbf{k}$-points in the Brillouin zone. The optimization (atomic positions and cell shape were allowed to change) of the low-T crystal structure was performed in the pseudopotential VASP code[18] with the same type of the exchange-correlation potential and taking into account SOC. $Cs-s$ and $W-p$ were treated as valence states. We used cutoff 700 eV and the $\mathbf{k}$-mesh $6\times6\times6$ for optimization. The maximal force in the converged structure was less than 1 meV/Å.

In agreement with Ref. [11], we find that the GGA+SOC in the proposed LT structure gives a strongly metallic ground state in a drastic contrast to experiment. Moreover, this state turns out to be magnetic, with small,
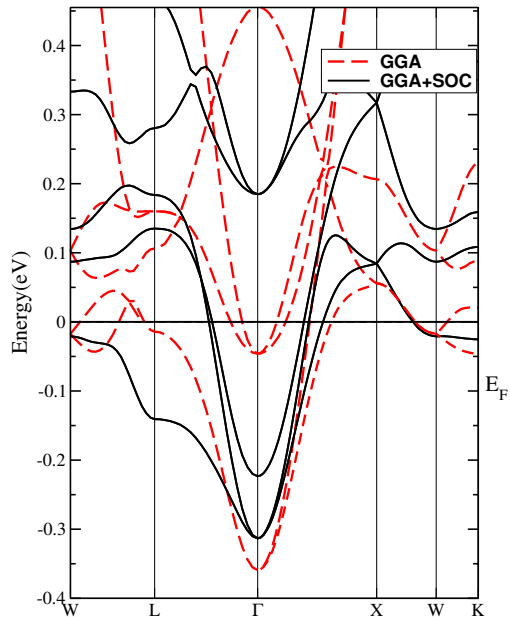


Figure 1: The band structure obtained for the HT phase in the GGA and GGA+SOC calculations. Positions of the high-symmetry points in the Brillouin zone are shown in Fig. 2.

but solid spin moments $m_s^{W1} \sim 0.19\mu_B$ and $m_s^{W2} \sim 0.13\mu_B$. While these moments are further partially reduced by orbital contributions $m_o^{W1} \approx m_o^{W2} \sim -0.05\mu_B$, they are still non-negligible, which again stresses discrepancy with the experimental data. Moreover, there are enormous atomic forces up to 0.8 eV/Å, which make this structure unstable in the GGA+SOC. As expected, including Hubbard correlations within the GGA+U+SOC (we used $U = 2$ eV and $J_H = 0.5$ eV) only worsens the situation, as moments begin to grow, while the system remains metallic.

In order to gain more insight into the physics of the LT phase we start by analyzing the band structure of the HT cubic phase. Without SOC there are five bands (Fig. 1) crossing the Fermi energy ($E_F$). Two bands with small dispersion cross $E_F$ in W-L, W-X and W-K directions, which results in a large density of states (DOS) at $E_F$ and electronic instability. There are also two bands crossing $E_F$ in the vicinity of the $\Gamma$ point. All these bands are mostly of the W $t_{2g}$ character.

The SOC dramatically modifies the band structure. The Fermi surface is considerably simplified, and becomes canonically semi-metallic. The unphysically large DOS is suppressed from $\sim15$ states/(eV f.u.) in nonmagnetic GGA to $\sim6$ states/(eV f.u.) in GGA+SOC. Two bands are crossing the Fermi level near $\Gamma$, and one near X, forming, respectively, two nearly degenerate electron pockets and three hole pockets per the reciprocal cell.
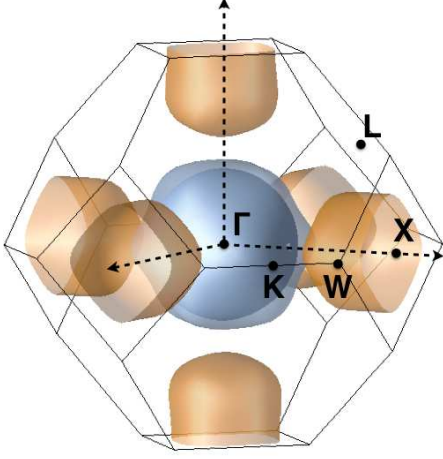
Figure 2: The Fermi surface as obtained in the GGA+SOC calculation for the high-temperature phase.
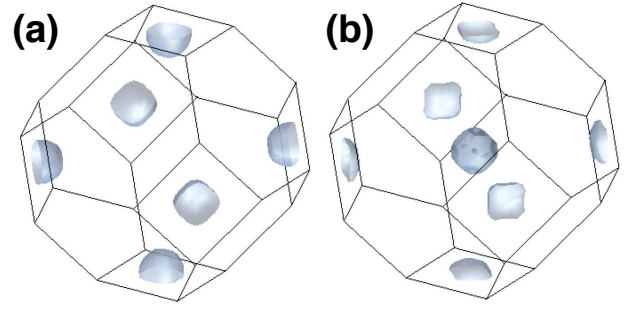


Figure 3: Real (a) and imaginary (b) parts of the noninteracting susceptibility $\chi_0(\mathbf{q})$ calculated from the high-T band structure. Isosurfaces with $\chi_0(\mathbf{q}) = 92\%\chi_0^{max}$ are shown.

The former are nearly spherical, and the latter are more like rounded parallelepipeds.

This topology is prone to various instabilities. The energy mismatch when the Fermi surfaces are shifted by the corresponding wave vector varies between 0 and ∼50 meV. Thus, energy can be gained by generating three simultaneous CDWs that fold all three hole pockets right upon the electron pockets. As long as the potential generated by the CDW is larger than $V \gtrsim 50$ meV, a gap of the order of $V$ will open, with a metal-insulator transition into a band insulator phase [27]. Finally, as discussed in the next session, arguably the most interesting instability this Fermi surface is conducive to is an unconventional superconductivity.

Experimentally, it is clear that the second option is realized in the actual material. Note that simultaneous condensation of the three CDWs in question quadruples, but not octuples the unit cell. From the fact that the coordinates of the X point of the Brillouin zone are $(2\pi/a, 0, 0)$ it is obvious that going from the FCC Bravais lattice with the wave vectors $[a/2, a/2, 0]$, $[a/2, 0, a/2]$ and $[0, a/2, a/2]$ to the conventional cell with $[a, 0, 0]$, $[0, a, 0]$ and $[0, 0, a]$ corresponds to three CDWs with the X,Y and Z wave vectors.

Another way to look at this issue is to calculate, as it is often done, [19] the noninteracting susceptibility, neglecting the $\mathbf{k}$-dependence of the matrix elements, defined as

$$\chi_0(\mathbf{q}) = \sum_{\mathbf{k},n,m} \frac{f_{\mathbf{k},n} - f_{(\mathbf{k+q}),m}}{\varepsilon_{\mathbf{k},n} - \varepsilon_{(\mathbf{k+q}),m}}, \qquad (1)$$

where $f$ and $\varepsilon_{\mathbf{k},n}$ are the occupation numbers and energies of the corresponding electronic states in the nonmagnetic GGA+SOC calculation, $n$ and $m$ enumerate bands. The results are presented in Fig. 3 and clearly show peaks of $\chi_0(\mathbf{q})$ at the X,Y, and Z points suggesting that the HT structure is unstable. While an account of the interaction and momentum matrix elements may change the shape of full susceptibility $\chi(\mathbf{q})$, it is unlikely to change the enhancement at the $X, Y, Z$ wave vectors, since it is driven by the phase space factor properly included already on the $\chi_0(\mathbf{q})$ level.

Keeping in mind these findings we performed calculation of the phonon spectra using a relativistic linear response DFT technique [20] and found pronounced instabilities with largest negative frequencies exactly at X point (see SM for details of the calculations and resulting phonon spectrum). Condensing of these two phone modes yields structures with the symmetry groups R32 and R3̄m, respectively. An arbitrary linear combination of these phonons gives the P4₁32 group. Optimizing the lattice in GGA+SOC within any of these groups leads to lower (compared to the reported structure) energies, but not insulating gaps. However, after checking possible subgroups of the P4₁32 group we found that further lowering the symmetry to P2₁2₁2₁ opens a gap, decreases the energy even further (by ∼135 meV/f.u. compared to that proposed in Ref. [11]) and is nonmagnetic, which agrees with experimental data.

There are 16 W atoms in the unit cell in the optimized structure. Half of these W form short W-W bonds (3.47Å), which results in an insulating ground state with four W bands below $E_F$, occupied by all 8 available $5d$ electrons of 16 W$^{5.5+}$ ions (details of the crystal structure together with corresponding band structure is given in SM). These short W-W bonds in no case should be considered dimers (typical distance in W dimers are ∼2.7Å[21]), but rather as a result of the CDW formation. This is a consequence of the pyrochlore lattice, where oxygen is in between of any two tungsten ions and prevents formation of real dimers. While average W-O bond distances for four inequivalent W in the optimized structure are nearly the same (∼ 1.95 Å), which agrees with results of Ref. [11], there is a certain charge modulation on W sites (see SM), consistent with formation of the CDW.

*Superconductivity.* Materials close to a CDW instability often harbor interesting superconductivity, which can either coexist with the CDW, or emerge upon suppression of the latter. As discussed below, doped CsW₂O₆

is a candidate for a highly unconventional superconducting state, predicted by Agterberg et al in 1999[22], but never observed (nor has any realistic candidate even been identified).

Let us briefly remind the reader of the essence of this work. Imagine the same Fermi surface as depicted in Fig. 2, but without the electron pockets. Let us further suppose that there is a pairing interaction that is stronger at small momenta. When sufficiently strong Coulomb interaction is present in the system (which is quite likely, given the small Fermi energy and thus small logarithmic renormalization), the superconductivity is optimized if the phase shift between the three inequivalent X-pockets is maximized, that is, equals $2\pi i/3$. Although not pointed out in the original paper[22], this state can be classified as "$d+id$", being a combination of the two states with the $e_g$ symmetry, $Y_{x^2-y^2} \pm iY_{3z^2-1}$, or $(Y_{2,2} + Y_{2,-2})/\sqrt{2} \pm iY_{2,0}$, the same combination was discussed by van den Brink and Khomskii in the context of the Jahn-Teller effect [23].

One may argue that if an electron pocket is present, it has to have gap nodes. This is true, but these nodes are only point nodes at the 8 directions $[\pm 1, \pm 1, \pm 1]$, and thus the mean square gap ($\sqrt{155/512} \approx 0.55$) is only 15% smaller than the maximal gap at $(\pm 1, 0, 0)$, namely $\sqrt{5/4\pi}$. Thus, this highly unconventional state is quite viable and may very well be realized in this material, if the high-temperature phase could be stabilized. Given that, as shown above, the metal-insulator transition in the real material is driven by a (spin-orbit induced) Peierls instability, the most natural way to stabilize the HT phase is to dope it in order to destroy nesting. Indeed a sister material, $CsTaWO_6$, occurs at all temperatures in a cubic phase isostructural to the HT phase of $CsW_2O_6$.[24]. This material is doped with 1/2 hole per $5d$ metal ion, that is to say, W and Ta occur in the $d^0$ configuration, so useless from the point of view of superconductivity. Synthesizing intermediate materials of the composition $CsW_{1+x}Ta_{1-x}O_6$, $0 < x < 1$, is more promising and must be feasible. One caveat is in place: as any other $d$−wave superconductivity, this $e_g + ie_g$ state would be sensitive to impurity scattering, so the unavoidable W-Ta disorder may suppress or entirely destroy this superconducting state. Other possibilities include (i) introducing Cs vacancies, (ii) partially replacing O with N, or (iii) applying pressure (in the latter case the nesting would likely be unchanged, but the elastic energy penalty for the Peierls transition would increase).

*Conclusions.* $CsW_2O_6$ appears to be a highly interesting material, harboring quite unusual and even intriguing physics. So far it has been barely studied experimentally and not investigated theoretically at all. We hope that our work will stimulate further research.

Our main results are as follows: a close inspection of the experimentally reported low-$T$ structure reveals that it cannot possibly open an insulating gap, and at least a twice larger cell is needed, and that this structure generates large forces in DFT, signaling that it is far from the lowest-energy structure. Examining the high-$T$ structure, which had been unambiguously established, we find that its fully-relativistic (spin-orbit coupling is absolutely essential) Fermi surface exhibits an amazingly simple semi-metal topology, with a good, well-visible in the calculated susceptibility, electron-hole nesting. This nesting makes the high-$T$ structure unstable against simultaneous formation of three charge density waves, running in the three orthogonal crystallographic directions, i.e. susceptible to such a rare phenomena as the 3D Peierls transition. Subsequent calculation of phonon spectrum demonstrates that the largest negative phonon frequencies are exactly at those points of the Brillouin zone, where the susceptibility diverges. The crystal structure obtained by the lattice optimization using eigenvectors of the lowest in energy phonon branches shows formation of short W-W bonds for half of W atoms in the unit cell. $CsW_2O_6$ in this structure was found to be insulating and nonmagnetic, fully consistent with available experimental data. Having demonstrated that the observed transition is nesting-driven and thus must be very sensitive to the band filling, we speculate that alloying with Ta should suppress the CDW state rather rapidly.

Finally, we note that the calculated topology of the Fermi surfaces (in the HT phase) is exactly the one required to realized an intriguing proposal of Gor'kov and his collaborators about a 3D $d$−wave state, which breaks the time reversal symmetry without being chiral, and can be characterized as a 3D version of the famous "$d + id$" state (which in this case becomes $e_g + ie_g$).

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[27] Note that this Fermi surface is topologically consistent with an excitonic insulator instability[25]. Since both CDW and $\mathbf{q} \neq 0$ excitonic insulator break the same symmetries and both can be diagrammatically described as instabilities in the particle-hole channel [26], we do not distinguish these in the forthcoming discussion.