Web links to the author's journal account have been redacted from the decision letters as indicated to maintain confidentiality.

Decision letter and referee reports: first round

Dear Prof Enderlein,

Thank you for submitting your manuscript, "Pressure-induced Anderson-Mott Transition in Elemental Tellurium", to Communications Materials. It has now been seen by 3 referees. You will see from their comments below that while they find your work of potential interest, some important points are raised that must be addressed. In particular, Reviewer #2 has serious concerns regarding the theoretical interpretation of your results and the nature (Lifshitz-like versus Anderson-Mott-like) of the quantum critical behaviour, which should be firmly established (possibly with additional data in the vicinity of the critical point) in order to support the claims of your manuscript. Furthermore, Reviewer #3 is requesting to clarify several technical points in order to substantiate the scientific soundness of your work. We would naturally expect the other requests and comments of the referees to be appropriately responded to, including their requests for further information and discussion.

We are interested in the possibility of publishing your study in Communications Materials, but would like to consider your response to these concerns in the form of a revised manuscript before we make a final decision on publication. We therefore invite you to revise and resubmit your manuscript, taking into account the points raised.

We are committed to providing a fair and constructive peer-review process. Please don't hesitate to contact us if you wish to discuss the revision in more detail.

When submitting your revised manuscript, please include the following:

-A rebuttal letter with a point-by-point response to each of the referee comments and a description of changes made. Please include the complete referee report in the rebuttal letter. Please note that the rebuttal letter must be separate to the cover letter to the editors.

-A marked-up version of the manuscript with all changes to the text in red colored font. Please do not include tracked changes or comments. Please select the file type ‘Revised Manuscript - Marked Up’ when uploading the manuscript file to our online system.

-A clean version of the manuscript. Please select the file type ‘Article File’.

-An updated Editorial Policy checklist, uploaded as a ‘Related Manuscript File’ type. This checklist is to ensure your paper complies with all relevant editorial policies. If needed, please revise your manuscript in response to these points. Please note that this form is a dynamic ‘smart pdf’ and must therefore be downloaded and completed in Adobe Reader. Clicking this link will download a zip file containing the pdf.

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** This url links to your confidential home page and associated information about manuscripts you may have submitted or be reviewing for us. If you wish to forward this email to co-authors, please delete the link to your homepage first **

We hope to receive your revised paper within three months; please let us know if you aren't able to submit it within this time so that we can discuss how best to proceed. If we don't hear from you, and the revision process takes significantly longer, we will close your file. In this event, we will still be happy to reconsider your paper at a later date, as long as nothing similar has been accepted for publication at Communications Materials or published elsewhere in the meantime.

We understand that due to the current global situation, the time required for revision may be longer than usual. We would appreciate it if you could keep us informed about an estimated timescale for resubmission, to facilitate our planning. Of course, if you are unable to estimate, we are happy to accommodate necessary extensions nevertheless.

Please do not hesitate to contact me if you have any questions or would like to discuss these revisions further. We look forward to seeing the revised manuscript and thank you for the opportunity to review your work.

Best regards,

Dr Aldo Isidori
Associate Editor
Communications Materials

Reviewers' comments:

Reviewer #1 (Remarks to the Author):

The reviewed article describes the results of experimental and theoretical studies of magnetotransport phenomena in the tellurium elementary semiconductor. The calculations were performed by DFT methods; a feature of low-temperature experiments is that they were performed under hydrostatic pressure. Tellurium is a gyrotropic crystal with strong spin-orbit interaction, which results in a special kind of valence band. The main goal of the work is to show that when the external pressure changes, the

metal-insulator transition occurs due to the restructuring of the band structure, i.e., it is the Lifshitz transition. The authors, in my opinion, achieved the goal and the article will be interesting for a wide circle of researchers. However, in my opinion, the Authors need to make a small addition about the odservation of the Lifshitz transition in other materials and thereby emphasize the difference between their results and other authors.

Reviewer #2 (Remarks to the Author):

The work deals with a very interesting topic, and the wide array of experiments goes quite a way towards presenting evidence for the claims made.

Whilst this is true, I find the theoretical interpretation to be incomplete and confusing enough to be problematic. Let me explain:

(1) The authors claim a Lifshitz-Anderson-Mott transition under pressure.Already from their DFT results, however, one would expect to have a Lifshitz criticality where the FS topology changes at Pc. In fact, this can best be seen if one performs a Ginzburg-Landau analysis, as done by Imada and coworkers around a decade ago. One would have a set of critical exponents therefrom. This is the first source of my concern: in absence of such an analysis, the authors associate the critical exponents to an Anderson-Mott mechanism. Why are these exponents NOT associated with Lifshitz quantum criticality, perturbed by disorder, at the outset? I strongly feel that the authors should consider this aspect before ruling this option out.

(2) if, as the authors themselves say, the transition occurs in tail states (assuming that the above scenario suggested as an alternative by me is invalid), coulomb interaction effects will be large. why is DFT, which neglects such effects altogether, to be trusted in such cases? In fact, I would have thought that the bad metal/ bad insulator state seen above 2K would be associated with proximity to localised states with k_(F)l = O(1). Such a state would be very far from DFT predictions.

(3) The English could be improved at various points. I found, disconcertingly, that quite a few statements were grammatically flawed. This would present problems to readers. I had to really read parts of the paper twice whilst refereeing it, and I urge the authors to improve this aspect.

(4) the quality of the fits used to extract critical exponents ta might be improved substantially by having a few more experimental points close to the claimed QCP. This is especially important in a situation where the criticality could be dominantly Lifshitz type, with additional subtleties due to disorder (see my critique (1) above), or a Mott-Anderson type (authors' claim): distinguishing between the two scenarios then becomes crucial, and this requires very reliable data close to the QCP.

To sum up, the study is very interesting in its conception and experimental execution. My issue with the

work is at the level of interpretation and, while their claim could ultimately remain valid, more analysis as I request above is necessary to settle the issue of a Lifshitz-like versus Anderson-Mott like transition. In absence of clarity on this aspect, their main message would lose its punch. I would be very interested in the ultimate outcome of this very interesting problem.

Reviewer #3 (Remarks to the Author):

The authors discuss the properties of elemental tellurium under pressure. By measuring the temperature dependence of conductivity (resistivity) under pressure they identify the phase transition around Pc=17.43 kbar. By analyzing the data and combining the DFT calculation, they conclude that the phase transition occurs from Anderson insulator to disordered metal with Lifshitz transition. The experimental data themselves seem to make some contribution to understanding of tellurium and the Lifshitz transition shown by the DFT calculation seems interesting. However, I could not understand some points, which prevents me from judging whether the whole story of the manuscript is scientifically valid. Hence, I cannot recommend publication in the current form of the manuscript.

Questions and comments are as follows.
Main points:
1. In the 8th page, the carrier density used in the DFT calculation is 1016 cm-3. However, this value is two orders of magnitude larger than the one by the Hall measurement. Is there any physical reason of the discrepancy? The main conclusion of this paper is the Lifshitz transition, which is derived from combined argument of the experimental data and the DFT calculation. However, the validity of the choice of the carrier density used in the DFT calculation is not clear.

2. In Fig.4, green area is referred to as critical phase. What is “critical phase”? I did not find the definition of the “critical phase” in the main text.

3. In Fig.4, black circles are plotted. Are these experimental data? If so, by which measurement are they obtained? Such explanation should be described in the main text and also in figure caption of Fig.4. The explanation of the red dashed line also seems to be remarked at least in the figure caption of Fig.4.

4. In Fig.4, there are two areas of spin-orbit metal. I could not understand why metallic regions are concluded from experimental data. For example, the resistivity at P=7.28 kbar in Fig.1a increases down to the lowest temperature. Furthermore, the energy gap opens as clearly shown in the inset of Fig.1b. However, authors assert the existence of the spin orbit metal at low temperatures in Fig.4 in this pressure region.

5. Description of introduction seems better to be improved. It was rather difficult to catch what is the main point of this paper. In abstract, authors described “historical and recent puzzling experimental findings”. If the result of this paper resolves historical and recent puzzles, it is better to be described

more clearly in the introduction.

Minor points:
6. In the 3rd line in introduction in the 2nd page, fig.3a & b appears as the first figure referred from the main text. Usually, figure number appears in order in the main text. Please check it.

7. In the last line in the 5th page, the characteristic temperatures of Ta1 and Ta2 are described as anomalous temperatures in the conductivity data. Although Ta1 and Ta2 are indicated with arrows in Fig.1c and 1d, it is hard to see what defines Ta1 and Ta2 in the data. In the main text, the definitions of Ta1 and Ta2 should be described clearly.

8. In Fig.4 the area denoted as VAI is “virtual Anderson Insulator”. What is the meaning of “virtual”? Is it different from Anderson insulator? Since Fig.4 provides the temperature-pressure phase diagram of tellurium, it seems better to use established terminologies familiar for readers (Anderson insulator is well known but virtual Anderson insulator is not).

Author responses: first round

We thank the the referees for their comments.

Answer to comments from referee 1

Comment referee 1:

The reviewed article describes the results of experimental and theoretical studies of magnetotransport phenomena in the tellurium elementary semiconductor. The calculations were performed by DFT methods; a feature of low-temperature experiments is that they were performed under hydrostatic pressure. Tellurium is a gyrotropic crystal with strong spin-orbit interaction, which results in a special kind of valence band. The main goal of the work is to show that when the external pressure changes, the metal-insulator transition occurs due to the restructuring of the band structure, i.e., it is the Lifshitz transition. The authors, in my opinion, achieved the goal and the article will be interesting for a wide circle of researchers. However, in my opinion, the Authors need to make a small addition about the observation of the Lifshitz transition in other materials and thereby emphasize the difference between their results and other authors.

We thank the referee for the positive response and for his/her suggestion that we should include additional material on the Lifshitz transition in other materials. We agree with this analysis, as it also addresses the critiques of the other referees. In order to clarify that tellurium undergoes a genuine Anderson-Mott insulator-to-metal phase transition (at fixed carrier density) that is nevertheless driven by pressure across a Lifshitz transition (which is different from a true Lifshitz metallic phase transition) we made the following changes:

1.) The last paragraph of the introduction now reads: "This study has identified and highlighted the importance of the quantum critical point in tellurium and provides an understanding of the ground state of high purity tellurium crystals. It also addresses the intriguing theoretical predictions on the possible emergence of topologically interesting phases in chiral non-centrosymmetric tellurium. Furthermore it demonstrates a unique scenario, in which pressure tunes an Anderson-Mott insulator-to-metal phase transition across a Lifshitz transition and therefore exhibits completely different characteristics from systems which undergo a true Lifshitz phase transition as in [27] and [28]."
2.) The second paragraph of the "Critical behaviour close and the quantum phase transition" section (section 2.3), now starts with "The respective Mott-Anderson transition coincides with the pressure induced Lifshitz transition in p-type tellurium [22, 26]. As will be established below, at the point of the Lifshitz transition the Fermi level is pushed below the mobility edge, leading to an Anderson-Mott quantum critical point."

Answer to comments from referee 2

Comments referee 2:

We thank the second referee for his/her comments, which address several important issues.

(1) The authors claim a Lifshitz-Anderson-Mott transition under pressure. Already from their DFT results, however, one would expect to have a Lifshitz criticality where the FS topology changes at Pc. In fact, this can best be seen if one performs a Ginzburg-Landau analysis, as done by Imada and coworkers around a decade ago. One would have a set of critical exponents therefrom. This is the first source of my concern: in absence of such an analysis, the authors associate the critical exponents to an Anderson-Mott mechanism.

Why are these exponents NOT associated with Lifshitz quantum criticality, perturbed by disorder, at the outset? I strongly feel that the authors should consider this aspect before ruling this option out.

We agree completely with the referee that one should analyse the data starting from the critical exponents of a genuine Lifshitz phase transition. However, what our study has shown is that tellurium undergoes instead a genuine Anderson-Mott insulator-to-metal transition that nevertheless coincides with a Lifshitz transition. At the point of change of the topology of the Fermi surface, the Fermi level is pushed to below the mobility edge, paving the way for the Anderson-Mott phase transition. This is different from a genuine metallic Lifshitz phase transition as the ones considered by Imada and co-workers. We have ruled out the possibility of true Lifshitz-type quantum fluctuations dominating the transition for the following reasons:

1.) On both sides of the transition, transport is dictated by quantum localization (VRH with small $_0$ on the insulating side, $= _0 + \sqrt{}$ on the metallic side). If the Lifshitz related fluctuations played a significant role, we would expect normal metallic behaviour on both sides of the transition, as the Lifshitz-related quantum fluctuations are causally related to the shape/topology of an existing Fermi surface.

2.) In the critical regime, we measure $= _0 + _3$, which is typical for the Mott-Anderson transition. We do not know which behaviour would be expected at the critical point in case of a neck-disrupting Lifshitz transition, but we know that we would expect a conductivity that decreases with increasing temperature, as neither thermally activated behaviour, nor quantum interference effects would be expected. Instead we would expect a power-law of the resistivity.

3.) However, one might still argue that the Lifshitz transition should manifest itself indirectly in the data. All our theoretical framework is based on the idea that this is not the case. How is this possible?
The answer lies in the fact that the bandwidth, and therewith the distance to the mobility edge, scales approximately linear over a small pressure range with the pressure. Therefore, the mathematical framework of the Mott-Anderson transition holds.

4.) However, we could still perform an analysis of critical exponents, just for the sake of the argument. We encounter some problems here, as it seems strange to associate the localization length in $_0$ with the length scale from the Lifshitz transition, which relates to the inverse of the Fermi-surface thickness at the neck-position. However, if we do that, we might expect a critical exponent $= _2$ of , as in Enderlein *et.al.* (2013), (now cited in the new version if the paper). This would lead to a $= 1.5$. Looking at fig. 2a), this is inconsistent with our data.

5.) Finally, it is possible to extract the critical exponent from the data and compare it to Imada's $= 4$. The universality relating the AM transition in $= 3$ to random-field magnets gives rise to a scaling description quite different from the $2 +$ cases considered by Imada. There are two crucial properties of the scaling for the AM transition in $= 3$:

   a. the first is the realization that the electron-electron interaction is renormalization group irrelevant at this transition in $= 3$ (see for example section VI-B.3 of *Quantum phase transitions in electronic systems*, by T. R. Kirkpatrick and D. Belitz, in Electron Correlations in The Solid State, ed. Norman H. March, Imperial College Press 1999). As a result, the frequency

mixing that produces independent dynamical exponentes z in $d = 2 + E$ is absent. Here, instead, the frequency plays the role of an external field that is conjugate to the order parameter and z is not independent, but is related to the exponents fi, 8, and v, via

$$z = \frac{8fi}{v}$$

b. the second concerns the scaling behaviour of transport coefficients. The diffusion coefficient obeys the homogeneity condition

$$D(t, T) = b^{2z} D\left(tbv, Tb^{z}\right)^{1}$$

where t -, 0 controls the proximity to the critical point. Since the diffusion coefficient is related to the static electrical conductivity one obtains

$$Q4,T) = tsF,(tT\ vz)$$

that is, $_{t,}$ in the critical region becomes a function of $\frac{T}{t_{yz}}$, rather than of T and t separately. According to Wegner's scaling in $d = 3$, this implies that, in the critical region the scaling function $F,$ for $t = 1$, far above the transition, is determined by

$$Q(T) \text{-} T^{\frac{1}{z}} \text{-} T^{\frac{1}{3}}$$

since $fi = v$ (Wegner's scaling) and $8 = 3$ (random-field magnet)
$z = 3$.

As we can see, the dynamical exponent z = 3 for the AM transition extracted from our data for the critical static conductivity is different from the one expected for a Lifshitz transition in correlated, topological Fermi-liquids, $z = 4$, where electronic correlations are not irrelevant, but marginally irrelevant.

Within the paper we have now added several sentences to address the concern:

1. The second paragraph of "Critical behaviour close and the quantum phase transition" now includes the sentence "As will be established below, at the point of the Lifshitz transition the Fermi level is pushed below the mobility edge, leading to an Anderson-Mott quantum critical point."
2. Moreover, the second paragraph of the discussion section now includes "It is important to note that, although the transition occurs due to a topological change of the Fermi surface, it is actually of the Anderson-Mott manifold and obeys all its universal characteristics. This becomes particularly clear, when recognizing that on both sides of the transition, transport is clearly dictated by quantum interference corrections and in the critical regime, the Anderson-Mott typical $\sigma=\sigma_0 + AT^{1/3}$ is observed. The universality between the Anderson-Mott transition in $d=3$ and random-field magnets \cite{Belitz1994Anderson-Mott} allows us to identify the dynamic exponent z, from the $AT^{1/z}$ critical behaviour which, according to Wegner's scaling, $z=\beta\delta/\nu$, for $\beta=\nu$ and $\delta=3$ \cite{Belitz1994Anderson-Mott}, should be fixed to $z=3$, in agreement with our data, and markedly different from the $z=4$ exponent expected from a \textit{true} Lifshitz phase transition. Furthermore, as the bandwidth scales roughly linearly with

pressure, we would expect the closeness to the mobility edge also scales linearly with pressure and therefore there is no overlying critical dependence from the \textit{true} Lifshitz transition."

(2)if, as the authors themselves say, the transition occurs in tail states (assuming that the above scenario suggested as an alternative by me is invalid), coulomb interaction effects will be large. why is DFT, which neglects such effects altogether, to be trusted in such cases? In fact, I would have thought that the bad metal/ bad insulator state seen above 2K would be associated with proximity to localised states with k_(F)l = O(1). Such a state would be very far from DFT predictions.

We thank the referee for this question. The referee is completely right in pointing out that Coulomb interaction effects are relevant. In fact, although Coulomb interaction is renormalization group irrelevant in d=3, it is necessary for the transition to occur and is crucial in providing the $()\sim^{3}$ critical behaviour seen in the data (see for example section VI-B.3 of *Quantum phase transitions in electronic systems*, by T. R. Kirkpatrick and D. Belitz, in Electron Correlations in The Solid State, ed. Norman H. March, Imperial College Press 1999). The terminology "Mott-Anderson transition" accounts for this fact.

As correctly pointed out by the referee, normal DFT (without enhancement) as a method does not allow to predict anything out of the single particle picture (SPP). However, we know from experimental data that the band bending in tellurium under pressure is real (see for example references 22 (Anzin, 1971) and 26 (Ideue, 2019)). As we use the DFT data only for qualitative statements, the calculations suffice the purpose of demonstrating that the (quantum interference and Coulomb driven) transition is tuned across an underlying transition of the topology of the Fermi surface.

In the new version of the manuscript, we explicitly acknowledge this fact in the abstract ("Such insulator to metal phase transition manifests itself in all measured physical quantities and their critical exponents are consistent with a scenario in which the often discussed pressure induced Lifshitz transition shifts the Fermi level to a position below the mobility edge, paving the way for a genuine Anderson-Mott transition.") and in the introduction ("Naturally, the disappearance of the double maximum coincides with a Lifshitz transition, drastically changing the density of states (DOS) at the Fermi level. Consequently, the Fermi level passes through the mobility edge and the material demonstrates a quantum phase transition from a Anderson-Mott insulator to a disordered metal."). We also want to point out that this point is central to the results in sections 2.2 and 2.3, when discussing the anomaly phase transition.

(3)The English could be improved at various points. I found, disconcertingly, that quite a few statements were grammatically flawed. This would present problems to readers. I had to really read parts of the paper twice whilst refereeing it, and I urge the authors to improve this aspect.

The paper is now proof-read by co-author SER, who is a native speaker. He found several typos, faulty expressions and small errors, which stand now corrected (marked in red as all the other, bigger changes).

(4)the quality of the fits used to extract critical exponents ta might be improved substantially by having a few more experimental points close to the claimed QCP. This is especially important in a situation where the criticality could be dominantly Lifshitz type, with additional subtleties due to disorder (see my critique (1) above), or a Mott-Anderson type (authors'claim): distinguishing between the two scenarios then becomes crucial, and this requires very reliable data close to the QCP.

Unfortunately, we cannot perform more measurements in general (due to the corona crisis) and specifically on the sample: tellurium samples are very brittle and after our measurement, the sample shows macroscopic changes in the form of cracks. Unfortunately, we do not have any way of performing more measurements within an acceptable time frame. However, we refer to our answer on point (1), as we believe that the case is now stronger.

Answer to comments from referee 3

We thank the third referee for his helpful comments:

1.In the 8th page, the carrier density used in the DFT calculation is 1016 cm-3. However, this value is two orders of magnitude larger than the one by the Hall measurement. Is there any physical reason of the discrepancy? The main conclusion of this paper is the Lifshitz transition, which is derived from combined argument of the experimental data and the DFT calculation. However, the validity of the choice of the carrier density used in the DFT calculation is not clear.

We thank the referee for his/her comment. The reason, why we chose to illustrate the Lifshitz transition assuming a charge carrier density 10^{16} cm^{-3} is that the Fermi surface is still sufficiently large to illustrate the Lifshitz transition without having to perform DFT calculations with a ridiculously large number of data points. As the DFT calculations serve mainly an illustrative purpose (it is clear that the same transition would occur for any other reasonable charge carrier density – only with a changed distance between the top of the band and the Fermi energy), we decided to perform the calculations for 10^{16} cm^{-3}. We have clarified this now in the related sentence. The respective part (third paragraph of section 2.3) reads:

"The Fermi level refers to a theoretical charge carrier density of $1 \cdot 10^{16} cm^{-3}$. This value is two orders of magnitude higher than the one we have measured by Hall. However, as the calculations serve mainly an illustrative purpose (meaning: they show the existence of a Lifshitz transition), we chose to use a higher charge carrier density. If we had used the measured charge carrier density, the necessary resolution for the DFT calculation would simply be too high to justify the time of calculation and moreover, the actual change of topology of the Fermi surface would be much more difficult to visually access in the figure."

2.In Fig.4, green area is referred to as critical phase. What is "critical phase"? I did not find the definition of the "critical phase" in the main text.

The term "critical phase" refers to the phase in which quantum fluctuations from quantum interference (between Anderson localization and weak localization), determine the transport properties. This phase is supposed to demonstrate $() = b + {}^{1}/_{3}$, which we measure indeed at 16.22 kbar (shown in the inset of fig. 1d). However, we naturally take some artistic freedom for the fig. 4, since we only have one pressure, where we measure the critical behaviour.

We did not change the text based on the referees comments, but we would like to mention that it says in the introduction "Close to the critical point, the system exhibits a conductivity varying with temperature as $\propto {}^{1}/_{3}$", in the legend of fig. 1 "The $\sigma \propto T$ 1/3 law indicates critical behavior.", in section 2.2 "As will become clearer further below, this coincides with the entrance in the critical regime, where the camel-back shaped top of the valence band, becomes a single maximum. Below the characteristic temperature T a2 at 16.22 kbar, the conductivity follows a T

1/3 -behavior (see inset of fig.1d), which is characteristic for the critical regime of the Anderson-Mott transition [36].”, and in the new version of the manuscript, the

section “2.3 Critical behaviour and the quantum phase transition” is solely dedicated to this issue.

3. In Fig.4, black circles are plotted. Are these experimental data? If so, by which measurement are they obtained? Such explanation should be described in the main text and in figure caption of Fig.4. The explanation of the red dashed line also seems to be remarked at least in the figure caption of Fig.4.

We thank very much for this comment. The points have been extracted from the position of the anomalies (which also mark the highest temperature for VRH and/or sqrt(T) behavior). This has been mentioned in the paper, but probably not with enough clarity. To change this, we have now added text below the legend of the figure (“The black circles mark the positions of the anomalies, which coincide with the temperature to which VRH and/or $\sigma = \sigma 0 + A \cdot T b$ is a good fit.”) and in the discussion (“(black circles represent the positions of the anomaly, which coincides with the respective change of slope in the R-T curves)”).

4. In Fig.4, there are two areas of spin-orbit metal. I could not understand why metallic regions are concluded from experimental data. For example, the resistivity at P=7.28 kbar in Fig.1a increases down to the lowest temperature. Furthermore, the energy gap opens as clearly shown in the inset of Fig.1b. However, authors assert the existence of the spin orbit metal at low temperatures in Fig.4 in this pressure region.

We thank very much for the comment and we are aware of the fact that the spin-orbit related delocalization in the low temperature regime in Anderson insulators is not common knowledge. As transport around the quantum phase transition is fully dictated from quantum corrections, at low temperature the spin-orbit interaction prevents a divergent resistivity for T->0. Therefore, the saturation of the resistivity corresponds to the conductivity associated with spin-orbit coupling. We have termed this “a spin-orbit metal” to avoid confusion, when recognizing that the resistivity does not diverge for $\rightarrow 0$. This is extensively discussed in the discussion section (and the supplementary material) in the paragraphs around equation (4).

5. Description of introduction seems better to be improved. It was rather difficult to catch what is the main point of this paper. In abstract, authors described “historical and recent puzzling experimental findings”. If the result of this paper resolves historical and recent puzzles, it is better to be described more clearly in the introduction.

We thank the referee for the comment. Due to journal guidelines, we have now heavily cut down the number of words in the abstract. The respective sentence has been removed, but the last sentence of the abstract now explicitly mentions “quantum oscillation measurements”, which have been performed previously in theoretically insulating tellurium crystals.

We thank the referee for this comment. The introduction underwent significant changes and we believe it to be much clearer. The last paragraph underlines the importance of the study.

6. In the 3rd line in introduction in the 2nd page, fig.3a & b appears as the first figure referred from the main text. Usually, figure number appears in order in the main text. Please check it.

We thank the referee for the comment. We have removed the reference to fig. 3, as it is not necessary for the understanding of the sentence.

7. In the last line in the 5th page, the characteristic temperatures of Ta1 and Ta2 are

described as anomalous temperatures in the conductivity data. Although Ta1 and Ta2 are indicated with arrows in Fig.1c and 1d, it is hard to see what defines Ta1 and Ta2 in the data. In the main text, the definitions of Ta1 and Ta2 should be described clearly.

The paragraph, where the anomalies are introduced now reads as follows: "At low temperatures, we observe two anomalies at characteristic temperatures T a1 and T a2 , which we determined by the position of a local maximum in the first derivative of ρ(T). For selected curves, the anomalies are marked in fig.1c & d by small black arrows (for a more detailed look on the resistivity data around the anomalies, see the supplementary material note 1). We believe the first anomaly to be the same, which has been reported before by Takita et. al. [14] for chemically pure samples with low hole concentrations."

8. In Fig.4 the area denoted as VAI is "virtual Anderson Insulator". What is the meaning of "virtual"? Is it different from Anderson insulator? Since Fig.4 provides the temperature-pressure phase diagram of tellurium, it seems better to use established terminologies familiar for readers (Anderson insulator is well known but virtual Anderson insulator is not).

The term "virtual" refers to the fact that the localization length, when approaching low temperatures, decreases to below the spin orbit relaxation length, which means that the Anderson insulator does not describe the ground state at zero Kelvin. We refer also to our answer to point 4 from the referee.

Further changes:

We recognized a double "chemically pure samples", thus we have changed one sentence in the introduction from "This is particularly important, since tellurium is naturally doped by vacancies, turning chemically pure samples into a p-type semiconductor and the resistivity curves generally show extrinsic behavior, even in chemically pure samples." to "This is particularly important, since tellurium is naturally doped by vacancies, turning chemically pure samples into a p-type semiconductor exhibiting extrinsic resistivity curves."

We changed the order of the sections, according to the journal guidelines and cut the "conclusions" section and included the text at the end of the discussion section

Following the journal guidelines, we included subsection titles in the "Results" section and all points where referred to the supplementary material now explicitly mention the respective note.

There are small changes over the whole paper, as we found double occurrences, typos and language errors (for example, "extent"->"extend", "historical"->"previous" etc.).

Decision letter and referee reports: second round

Dear Professor Enderlein,

Thank you for submitting your manuscript, "Pressure-induced Anderson-Mott Transition in Elemental Tellurium", to Communications Materials. Please accept our sincere apologies for the unusual delay in reaching a decision on your manuscript. We were hoping to receive a report from one of the referees (Reviewer #2) who initially reviewed your paper, but unfortunately the referee did not submit their report in due time.

Your manuscript has now been seen by 2 of our original referees, whose comments are appended below. You will see that while they find your work very much improved, Reviewer #3 has still some important concerns regarding the definition of the various 'phases' (or in some cases, 'regimes', as the referee suggests) that appear in the phase diagram of Fig. 4.

We are interested in the possibility of publishing your study in Communications Materials, but would like to consider your response to these concerns in the form of a revised manuscript before we make a decision on publication. We therefore invite you to revise and resubmit your manuscript, taking into account all the points raised.

We are committed to providing a fair and constructive peer-review process. Please don't hesitate to contact us if you wish to discuss the revision in more detail.

When submitting your revised manuscript, please include the following:

-A response letter with a point-by-point reply to each of the referee comments and a description of changes made. Please include the complete referee report in the response letter. Please note that the response letter must be separate to the cover letter to the editors.

-A marked-up version of the manuscript with all changes to the text in a different colored font. Please do not include tracked changes or comments. Please select the file type 'Revised Manuscript - Marked Up' when uploading the manuscript file to our online system.

-A clean version of the manuscript. Please select the file type 'Article File'.

-An updated Editorial Policy checklist, uploaded as a 'Related Manuscript File' type. This checklist is to ensure your paper complies with all relevant editorial policies. If needed, please revise your manuscript in response to these points. Please note that this form is a dynamic 'smart pdf' and must therefore be downloaded and completed in Adobe Reader. Clicking this link will download a zip file containing the pdf.

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We understand that due to the current global situation, the time required for revision may be longer than usual. We would appreciate it if you could keep us informed about an estimated timescale for resubmission, to facilitate our planning. Of course, if you are unable to estimate, we are happy to accommodate necessary extensions nevertheless.

Please do not hesitate to contact me if you have any questions or would like to discuss these revisions further. We look forward to seeing the revised manuscript and thank you for the opportunity to review your work.

Best regards,

Dr Aldo Isidori
Associate Editor
Communications Materials

Reviewers' comments:

Reviewer #1 (Remarks to the Author):

I asked the Authors to add a small section on the observation of the Lifshitz transition in other materials. Corresponding changes were made to the text. These changes, in my opinion, improve the content of the article.

Reviewer #3 (Remarks to the Author):

The authors have responded to most of the points I have raised. The revised manuscript is much more improved. Hence, I feel the manuscript will be acceptable, if the following points are resolved.

2. In the clean system without disorder, it is currently a critical issue whether quantum critical "phase" but not quantum critical point exists. If I understand the author's reply correctly, the green area in Fig.4 is a critical regime where quantum fluctuation gives rise to T^1/3 behavior in the conductivity. In the clean system, the regime where physical quantities such as resistivity, magnetic susceptibility, and specific heat show the critical temperature dependences in the temperature-pressure phase diagram, similar to Fig.4. However, it is not called critical phase but is called critical regime. To identify the existence of the "phase", the data in this manuscript seem not enough (pressure width of about 2kbar is indicated by only one set of black data points at T~1.2 K in Fig.4). Furthermore, it is unclear whether the VAI phase and DM phase is divided intrinsically by a single line but is smeared out by extrinsic factors such as experimental error and/or material condition, giving rise to a certain width of pressure.
Hence, it seems better to use critical "regime" but not critical "phase" for describing the green area in Fig4 in the main text. Otherwise many researchers would be confused.

3. In the first report, I commented that explanation of the red dashed line should be remarked at least in the figure caption in Fig.4. However, I neither found it in the revised manuscript nor in the author's reply.

4. In the sense that resistivity does not diverge for the zero temperature limit, author call it spin orbit metal from the viewpoint of the Anderson localization. However, although the resistivity does not diverge, the data shown in Fig.1a (for example at P=7.28 kar) increases toward the low temperature to reach about 4.7 Ohmcm. The band gap about 0.23 eV also opens as shown in Fig.1b. Therefore, I am still afraid to call this low-temperature limit "metal" practically, which may cause confusion for readers by literal interpretation of Figs.1a and 1b.

8. If author wishes to use "virtual Anderson insulator", the meaning of the virtual Anderson insulator is better to be explained in the main text and in the caption of Fig.4.

Author responses: second round

We thank the first referee for his positive comment.

Answer to comments from referee 2

In the clean system without disorder, it is currently a critical issue whether quantum critical "phase" but not quantum critical point exists. If I understand the author's reply correctly, the green area in Fig.4 is a critical regime where quantum fluctuation gives rise to T^1/3 behavior in the conductivity. In the clean system, the regime where physical quantities such as resistivity, magnetic susceptibility, and specific heat show the critical temperature dependences in the temperature-pressure phase diagram, similar to Fig.4. However, it is not called critical phase but is called critical regime. To identify the existence of the "phase", the data in this manuscript seem not enough (pressure width of about 2kbar is indicated by only one set of black data points at T~1.2 K in Fig.4). Furthermore, it is unclear whether the VAI phase and DM phase is divided intrinsically by a single line but is smeared out by extrinsic factors such as experimental error and/or materialcondition, giving rise to a certain width of pressure.

Hence, it seems better to use critical "regime" but not critical "phase" for describing the green area in Fig4 in the main text. Otherwise many researchers would be confused.

We thank the referee for pointing out this wrong use of nomenclature. We have now changed the term "critical phase" to "critical regime"

In the first report, I commented that explanation of the red dashed line should be remarked at least in the figure caption in Fig.4. However, I neither found it in the revised manuscript nor in the author's reply.

We apologize, as we had included the information on the meaning of the black markers without explicitly mentioning the red dashed line. This is now fixed (see caption fig. 4).

In the sense that resistivity does not diverge for the zero temperature limit, author call it spin orbit metal from the viewpoint of the Anderson localization. However, although the resistivity does not diverge, the data shown in Fig.1a (for example at P=7.28 kar) increases toward the low temperature to reach about 4.7 Ohmcm. The band gap about 0.23 eV also opens as shown in Fig.1b. Therefore, I am still afraid to call this low-temperature limit "metal" practically, which may cause confusion for readers by literal interpretation of Figs.1a and 1b.l".

We thank the referee for pointing out the confusion. We have now changed the nomenclature within the paper. The term "spin-orbit metal" has been removed and we have now substituted it by "delocalization as a consequence of the spin-orbit interaction" and other expressions (depending on the context).

If author wishes to use "virtual Anderson insulator", the meaning of the virtual Anderson insulator is better to be explained in the main text and in the caption of Fig.4.

Since we do not speak of a "spin-orbit metal" in the new version of the paper the "virtual" becomes obsolete. Thus, we now call the phase "Anderson insulator".

Decision letter and referee reports: third round

Dear Professor Enderlein,

Your manuscript titled "Pressure-induced Anderson-Mott Transition in Elemental Tellurium" has now been seen again by Reviewer #3 and by a new Reviewer #4, who was contacted in order to verify that your rebuttal to Reviewer #2 was convincing. Their comments appear below. In light of their advice I am delighted to say that we are happy, in principle, to publish a suitably revised version in Communications Materials under the open access CC BY license (Creative Commons Attribution v4.0 International License).

We therefore invite you to take into account the final small suggestion from Reviewer #4 (edit to the caption of Fig.4). At the same time we ask that you edit your manuscript to comply with our journal policies and formatting style in order to maximise the accessibility and therefore the impact of your work.

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We hope to hear from you within two weeks; please let us know if the process may take longer.

Best regards,

Dr Aldo Isidori
Associate Editor
Communications Materials

REVIEWERS' COMMENTS:

Reviewer #3 (Remarks to the Author):

I have read author's reply and confirmed that my concerns and suggestions are addressed.

Reviewer #4 (Remarks to the Author):

Please see the attached report.

Referee report for manuscript "Pressure-induced Anderson-Mott Transition in Elemental Tellurium" by Oliveira at el.

I have read the latest revision of the manuscript as well as the reply of the authors to the comments of all referees. I have paid particular attention to the reply of the authors to the comments of referee 2. This referee has raised two important points: (1) the fact that the authors classify the pressure-induced phase transition which they observe as a Anderson-Mott transition (and not a conventional Lifshitz transition, perturbed by disorder), and (2) the validity of DFT calculations in this context. As far as the first point is concerned, in their reply the authors give a number of arguments for the Anderson-Mott scenario which, in my opinion, are very convincing. Moreover, in the reply to (2) the authors emphasize that the use DFT results only for qualitative statements, which I also find acceptable.

My overall impression is that this a very interesting work. I also think that in Section 3 the authors analyze their data with great care in the light of available theory for the conductivity of disordered electrons. I therefore recommend publication of this work in Communications Materials.

Just a small comment: in the caption of Fig.4 the authors use the abbreviation VA for the phase which is labelled by AI in the figure; I suggest to replace VA by AI in the caption.