Pressure induced gap closing and metallization of MoSe$_2$ and MoTe$_2$

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Abstract

Layered molybdenum dichalcogenides are semiconductors whose gap is controlled by delicate interlayer interactions. The gap tends to drop together with the interlayer distance, suggesting collapse and metallization under pressure. We predict, based on first principles calculations, that layered semiconductors 2H$_c$-MoSe$_2$ and 2H$_c$-MoTe$_2$ should undergo metallization at pressures between 28 and 40 GPa (MoSe$_2$) and 13 and 19 GPa (MoTe$_2$). Unlike MoS$_2$ where a 2H$_c$ → 2H$_a$ layer sliding transition is known to take place, these two materials appear to preserve the original 2H$_c$ layered structure at least up to 100 GPa and to increasingly resist lubric layer sliding under pressure. Similar to metallized MoS$_2$ they are predicted to exhibit a low density of states at the Fermi level, and presumably very modest superconducting temperatures if any. We also study the β-MoTe$_2$ structure, metastable with a higher enthalpy than 2H$_c$-MoTe$_2$. Despite its ready semimetallic and (weakly) superconducting character already at zero pressure, metallicity is not expected to increase dramatically with pressure.

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I. INTRODUCTION

Transition Metal Dichalchogenides (TMDs) are well known and long characterized compounds. They possess a layered crystal structure consisting of MX$_2$ (M-transition metal, X-chalcogen) XMX composite triatomic layers where the transition metal monoatomic layer is sandwiched between two layers of chalcogen atoms. The layers consisting of covalently bonded atoms are only weakly coupled by partly van der Waals interactions, resulting in highly anisotropic properties. By analogy with graphite, their structure based on independently stable, relatively unreactive triatomic layers which can be mutually sheared is probably related to the functioning of some materials such as MoS$_2$ and MoSe$_2$ as lubricants. It opens at the same time the way to a rich polytypism, due to various possible relative stackings of the layers. Much initial interest in bulk materials has been driven by their electronic properties, including insulator, semiconductor, metal, charge-density-wave (CDW) material, and superconductor – properties that can also be modified by intercalation. More recently, focus shifted to the exfoliated monolayers, similar to graphene. Owing to removal of interlayer interactions a monolayer has, unlike the bulk material, a larger and direct band gap, features which in MoS$_2$ make it of interest for optoelectronics (Refs. 3, 4, 5, 6, 7).

On the opposite front, it is possible to modify the properties of bulk TMDs by external hydrostatic pressure which can in principle cause structural as well as electronic phase transitions. In Ref. 9 2Hc-MoSe$_2$ was compressed up to 35.9 GPa and studied by X-ray diffraction but no structural transition was reported. At normal conditions MoS$_2$, MoSe$_2$ and MoTe$_2$ are semiconductors with indirect energy gaps of about 1.29 eV, 1.1 eV and 1.0 eV, respectively.

The behaviour of MoS$_2$ under pressure is now well understood. Its resistivity decreases with pressure suggesting possible metallization at high pressure. While that possibility is confirmed by calculations it was also theoretically found that the initial 2H$_c$ structure (hexagonal, space group $P6_3/mmc$) at zero pressure should undergo near 20 GPa a pressure induced structural transition to 2H$_a$ (the same space group $P6_3/mmc$), the structure typical of e.g. NbS$_2$. That result explained some previously mysterious X-ray diffraction evidence and Raman scattering data and was also recently confirmed experimentally. Both MoS$_2$ phases were predicted to metallize at the same pressure region where the structural transition takes place, 2H$_c$ at 25 GPa and 2H$_a$ at 20 GPa – an electronic result not yet investigated.
by experiments.

The behaviour of MoS$_2$ suggests the possibility that pressure-induced gap closing similar to that of MoS$_2$ might occur in the similar materials MoSe$_2$ and MoTe$_2$. The experimental electrical resistivity of MoSe$_2$ under pressure appears to be controversial. In Ref.$^{10}$ a sudden resistivity drop was found at 4 GPa, with no interpretation provided. In more recent work Ref.$^{15}$ resistivity was studied up to 8 GPa and found to decrease smoothly upon compression with no sudden drop.

For the next member of this group, MoTe$_2$, also semiconducting in its 2H$_c$ room temperature, zero pressure stable form ($\alpha$-MoTe$_2$), the pressure dependence of resistivity is not known. High temperature is known to induce a structural transition to a new $\beta$-MoTe$_2$ phase$^{10}$ (monoclinic, space group $P2_1/m$), still a layered structure with additional modulation of structure inside the layers, so that the Mo atoms now present a distorted octahedral coordination rather than the trigonal prismatic one of 2H$_c$.$^{17}$ Interestingly the $\beta$-phase is metallic at zero pressure. The transition from $\alpha$- to $\beta$-MoTe$_2$ occurs by raising temperature to 900 °C (Ref.$^{16}$) but the new structure survives in a metastable state upon cooling down to room temperature – or even to cryogenic temperature where it reportedly shows superconductivity.$^{1}$ No high-pressure data appear to be available for either $\alpha$- or $\beta$-MoTe$_2$, and we can therefore only rely on theory concerning their structural and electronic behaviour in that regime.

Here we present first principles calculations based on density functional theory (DFT) demonstrating the effect of high pressure on bulk transition metal dichalcogenides MoSe$_2$ and MoTe$_2$, focusing both on the evolution of crystal structure and of electronic properties. We first of all will describe in the next section the technical details of DFT calculations. The following section will present our predicted evolution of crystalline and electronic structure, predicting the absence of structural transformations, surprising in view of the initial analogy to MoS$_2$, and a semiconductor-band overlap metal transition for both MoSe$_2$ and MoTe$_2$ upon compression. After a discussion of similarities and differences with MoS$_2$, in particular of the similarly poor metallic properties at high pressure, the last section will summarize our findings and draw conclusions.
II. CALCULATION METHOD

We follow well established understanding of, and specifically our own fresh experience with layered TMDs. Straight density functional total energy and structural calculations, quite delicate and uncertain at zero pressure due to large effects caused by the otherwise weak long-range interlayer dispersion van der Waals (vdW) forces which are beyond simple DFT, become much more reliable and predictive at high pressures, where vdW corrections become unnecessary. The case of MoS$_2$ had been particularly instructive in this respect,
showing that whereas the calculated zero-pressure c-axis interlayer spacing with the simple PBE exchange-correlation functional (no vdW) was as expected larger than experiment, it improved substantially at 5 GPa, turning extremely close to experiment at 10 GPa and upwards. Assuming, as is very reasonable, the same to hold for MoSe$_2$ and MoTe$_2$, we used no vdW correction and restricted our calculations to pressures of 10 GPa and higher, with no attempt to explore the more delicate and less interesting low pressure region. In order to increase the dependability of our predicted metallization pressures, we also repeated the electronic structure calculations (with PBE optimized structures, which are trustworthy) with the HSE06 functional which, contrary to PBE, overestimates band gaps and therefore metallization pressures too. The HSE06 calculations were used to establish an upper bound to the semiconductor-metal transition pressure. We employed the Quantum ESPRESSO package$^{19}$ for structural optimization and calculation of electronic properties. We used scalar relativistic pseudopotentials$^{26}$ and similarly to Ref.$^{11}$ we employed a PBE exchange-correlation functional$^{20}$ with cutoff of 950 eV. For 2H$_c$ structures we used the six-atom unit cell and $17 \times 17 \times 5$ Monkhorst - Pack$^{21}$ (MP) $k$-point sampling grid for relaxations and $24 \times 24 \times 8$ MP grid for electronic DOS calculations. For the $\beta$-MoTe$_2$ structure we used the unit cell with 12 atoms and $k$-points grids $7 \times 15 \times 5$ and $12 \times 24 \times 6$ for relaxation and DOS calculations, respectively. Spin-orbit coupling was not included in the calculation of total energy and structural optimizations, to which it contributes only in second order. We instead carried out test calculations to check the impact of spin-orbit on metallization pressures but found it to be also negligible. In all results presented below spin-orbit interaction is therefore omitted. Hybrid functional calculations employing the HSE06 functional were performed with norm-conserving pseudopotentials.$^{27}$ Zero temperature and neglect of zero-point energy contributions were assumed throughout.

A series of PBE calculations were carried out at increasing pressures from 10 GPa upwards, with at each pressure a full structural relaxation aimed at identifying the minimum enthalpy structure, its electronic band structure, and their pressure evolution.
III. RESULTS

A. MoSe$_2$

We performed a compression of the 2H$_c$-MoSe$_2$ unit cell up to 130 GPa and calculated the pressure dependence of the lattice parameters $a$ (intra-layer), and $c$ (inter-layer) (Fig. 2). For comparison we show in the same figure the experimental data extracted from X-ray diffraction patterns in Ref.\textsuperscript{9}. As can be seen the agreement is excellent especially at pressures beyond 15 GPa, which justifies \textit{a posteriori} the use of PBE functional without vdW corrections, as was also the case in MoS$_2$\textsuperscript{11}.

![Graph showing pressure dependence of lattice parameters](image)

FIG. 2: Pressure dependence of the calculated lattice parameters $a$ (upper panel) and $c$ (lower panel) of 2H$_c$-MoSe$_2$ together with experimental data from Ref.\textsuperscript{9}.

Results also agree with experiment Ref.\textsuperscript{9} in MoSe$_2$ indicating no structural changes and the stability of the 2H$_c$ zero pressure structure of MoSe$_2$ at least up to 35.9 GPa. In order to check whether any transition could take place at a higher pressure than this, it would
be necessary in the future to conduct some kind of structural search. Limiting ourselves to explore the simple possibility of a transition to the 2H_a structure, we calculated the enthalpies of both 2H_a and 2H_c phases of MoSe_2 up to 130 GPa. Fig. 3 shows the enthalpy difference between the two phases. Unlike the case of MoS_2 where the enthalpies cross and the 2H_a polytype became more stable around 20 GPa, here the enthalpy difference actually increases with pressure, thus reinforcing the stability of the 2H_c structure. The slope of the enthalpy difference with increasing pressure (Fig.3 and Fig.2 in Ref.11) is equal to the volume difference between the respective phases and the behaviour of MoSe_2 and MoTe_2 is just the opposite of MoS_2: e.g. at p=20 GPa the volume of the unit cell of the 2H_a phase compared to the 2H_c one is larger in MoSe_2 and MoTe_2 by 0.2 % and 1.4 %, respectively, while in MoS_2 it is smaller by 1 %. The layer-sliding structural transition observed in MoS_2 therefore is not expected to occur in MoSe_2 – and, as we shall see further down, neither is it in MoTe_2.

We can rationalize the reason for that difference of behaviour between MoSe_2 or MoTe_2 and MoS_2 based on simple considerations of interlayer Mo-Mo metallic bonding. We first note that only in the 2H_a structure the Mo atoms in nearest layers are vertically on top of one another, whereas they are staggered and chemically far away in 2H_c. The 2H_a structure can be energetically favored if it can take advantage of d-electron propagation and metallicity along the c-axis, such as is the case in NbS_2, NbSe_2, and high pressure MoS_2. In MoSe_2 and MoTe_2, due to the larger radius of anions, the interlayer Mo-Mo distances are larger, e.g., by about 0.25 Å in MoSe_2 than in MoS_2. That makes interlayer d-electron propagation energetically less important in MoSe_2 leaving anion-anion repulsive forces in control of the enthalpy balance and finally favoring 2H_c over 2H_a.

Having thus characterized the pressure evolution of the atomic structure, we can examine that of electronic properties, in particular the pressure induced closing of band gap and metallization. The calculated PBE band structure is shown in Fig.4 for 2H_c-MoSe_2 at $p = 10$ GPa and $p = 30$ GPa. The gap decreases with pressure at the rate of 0.026 eV/GPa. At $p = 10$ GPa there still is an indirect band gap of 0.47 eV with the valence band top at the Γ point and the conduction band bottom at some point $Q$ close to the midpoint between Γ and $K = \frac{1}{3}b_1 + \frac{1}{3}b_2$, where $b_1, b_2$ are reciprocal lattice vectors and $|\Gamma K| = \frac{4\pi}{3a}$.

At $p = 30$ GPa the band gap is already closed and the valence and conduction bands exhibit a tiny overlap. Since the PBE approximation certainly does not overestimate the band gap, our calculation suggests that metallization of 2H_c-MoSe_2 at lower pressures than
FIG. 3: Pressure dependence of the enthalpy difference between the $2H_a$ and $2H_c$ structures of MoSe$_2$ and MoTe$_2$, respectively. Note the increase with pressure, indicating increased stability of $2H_c$ in both materials, unlike MoS$_2$ where $2H_a$ prevails at high pressure.$^{11}$

30 GPa is unlikely. This is compatible with the more recent resistivity data of Ref.$^{15}$ (which appear to correct earlier results$^{10}$ which had suggested a transition at 4 GPa for which there is no supporting evidence). In Fig.3 we show our predicted pressure dependence of the band gap which shows metallization by band overlap in MoSe$_2$ at $P_{met}$ = 28 GPa. Following band overlap, $2H_c$-MoSe$_2$ turns semimetallic with a low density of states at the Fermi level, as shown by Fig.6 at $p$ = 30 GPa. To establish an upper bound for the metallization pressure we then performed calculations using the same structures, but the HSE06 hybrid functional$^{22}$ in place of PBE and found the gap closing at 40 GPa. Since this approximation is known to overestimate the band gap, we conclude that MoSe$_2$ metallizes at pressure between 28 and 40 GPa.

Since for an indirect band gap semiconductor the exciton binding energy $E_B$ remains finite right up to $P_{met}$, there is in principle the possibility upon gap closing to realize a so-called excitonic insulator state. That is a kind of charge-density-wave or spin-density-wave state with wavevector $Q$ theoretically predicted long ago in Ref.$^{23}$. In a narrow range of pressures immediately below $P_{met}$ the semiconducting gap becomes small enough to be comparable with the exciton binding energy $E_B$, expected here to be of order of 10 meV. Given a gap reduction rate of 26 meV/GPa, this means that the excitonic state could exist in a narrow pressure range of about 4 kbar below $P_{met}$. The DFT-PBE electronic structure approximation does not treat properly the nonlocal exchange which is essential for the description of excitons, and thus it does not describe excitonic insulators states. Therefore we cannot make a quantitative prediction of the relevant portion of the pressure phase.
diagram and we must limit ourselves to a qualitative statement. The possible realization of this interesting state in MoS$_2$ was proposed in Ref.$^{11}$, but the structural transformation occurring at a pressure close to metallization presents a fatal complication in that system. From this point of view MoSe$_2$ (and as we shall see also MoTe$_2$), structurally stable lattice in the metallization region, appears to be a more suitable system to search for an excitonic insulator state.

**FIG. 4:** Band structure of 2H$_c$-MoSe$_2$ at $p = 10$ GPa (upper panel) and $p = 30$ GPa (lower panel).

B. MoTe$_2$

Compared with 2H$_c$-MoSe$_2$, there is much less experimental work for 2H$_c$-MoTe$_2$ ($\alpha$-form), and we are not aware of either structure or resistivity data under pressure, and our results represent a first theoretical exploration. We carried out the same calculation protocol as for for 2H$_c$-MoSe$_2$: total energy calculation, structural relaxation, enthalpy calculation, band structure and gap calculation. The calculated structural data are shown in Fig.$^7$ Here too
the 2H$_c$ structure remains stable under pressure, at least with respect to a transformation to 2H$_a$. The enthalpy difference stabilizing 2H$_c$ over the 2H$_a$ structure shown in Fig. 3 is here even stronger than in MoSe$_2$, in agreement with our earlier explanation involving the volume difference between the phases and the larger radius of Te anions relative to Se.
FIG. 7: Pressure dependence of the calculated lattice parameters $a$ (upper panel) and $c$ (lower panel) of 2H$_c$-MoTe$_2$.

Fig. 8 shows the band structure of 2H$_c$-MoTe$_2$. Here we took special care to verify that spin-orbit interaction has no major effect on the states in the vicinity of the Fermi level. At 10 GPa there is still a small but finite band gap. At 13 GPa band overlap has already taken place between the valence band top, now slightly displaced from $\Gamma$, and the conduction band bottom which has two nearly degenerate minima - one again close to midpoint $Q$ between $\Gamma$ and $K$ points and another one at the $K$ point. Thus even in 2H$_c$-MoTe$_2$ there could be a narrow excitonic insulator phase just below the metallization pressure; however the CDW or SDW condensate wavevector is less straightforward to predict. Fig. 9 shows the electronic density of states at 10 and 30 GPa and one can see that even at 30 GPa, more than twice of the metallization pressure, the electronic DOS remains rather low, indicating semi-metallicity. Here again we performed a hybrid functional calculation and found gap closing at 19 GPa, thus placing the metallization pressure of 2H$_c$-MoTe$_2$ between 13 and 19 GPa.
Finally we studied the metastable $\beta$-form of MoTe$_2$ (Fig. 10) which is already metallic at zero pressure. The enthalpy of this form at 20 GPa is higher by 0.12 eV/(MoTe$_2$ group) than that of the 2H$_c$ form. In order to check how the metallicity of this phase evolves with pressure we compressed and relaxed this metastable structure to 20 and 40 GPa and recalculated electronic DOS (Fig. 11). The band structure at 40 GPa is also shown in Fig. 11. Comparing the DOS under pressure to that calculated for the experimental cell at normal conditions (from Ref. 17) we see that the effect of pressure again does not raise much the DOS at the Fermi level. This suggests that pressure is not a likely tool for a major increase of metallicity, and of BCS superconductivity, of $\beta$-MoTe$_2$.

IV. CONCLUSIONS

The structural and electronic properties of MoSe$_2$ and MoTe$_2$ are studied theoretically under high pressure. Unlike MoS$_2$, these TMD layered compounds are not prone to layer
sliding transition from 2H\textsubscript{c} to the 2H\textsubscript{a} polytype. Since MoSe\textsubscript{2} is also a good lubricant as is MoS\textsubscript{2},\textsuperscript{24} one can conclude that easy interlayer sliding in the high pressure pristine crystals may not be directly related to the lubricity shown by the technical emulsions based on these materials. Based on DFT-PBE calculations both compounds are predicted to metallize via closing of an indirect gap and consequent band overlap at pressures between 28 and 40

FIG. 9: Density of states per unit cell of 2H\textsubscript{c}-MoTe\textsubscript{2} at \( p = 10 \) GPa and \( p = 30 \) GPa.

FIG. 10: Structure of the \( \beta \)-form of MoTe\textsubscript{2} (a) and its I. Brillouin zone (b).
FIG. 11: Band structure of $\beta$-MoTe$_2$ at $p = 40$ GPa (upper panel) and density of states (per unit cell) at $p = 20$ GPa and $p = 40$ GPa and for the experimental unit cell at normal conditions (lower panel). In the DOS graph the Fermi energy is at zero.

GPa (2H$_c$-MoSe$_2$) and 13 and 19 GPa (2H$_c$-MoTe$_2$). Beyond the metallization point they should behave as semi-metals, retaining a low density of states at the Fermi level. Even in the metastable $\beta$-MoTe$_2$ phase, which is metallic already at zero pressure, compression does not appear to increase metallicity too much. Neither MoSe$_2$ nor MoTe$_2$ seem therefore likely, in their pristine non-intercalated state, to become good BCS superconductors in the range of pressures considered. Weak superlattice structural and electronic extra Bragg spots should be looked for just below the metallization pressure, with their possible presence providing evidence of an excitonic insulator state or CDW phase. In that case, enhanced superconductivity could arise in the metallic phase following the CDW at higher pressures, as seen for example in 1T-TiSe$_2$.\footnote{125}
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