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Carrier and strain tunable intrinsic magnetism in two-dimensional MAX₃ transition metal chalcogenides

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We present a density functional theory study of the carrier-density and strain dependence of magnetic order in two-dimensional (2D) MAX₃ (M= V, Cr, Mn, Fe, Co, Ni; A= Si, Ge, Sn, and X= S, Se, Te) transition metal trichalcogenides. Our ab initio calculations show that this class of compounds includes wide and narrow gap semiconductors, metals, and half-metals, and that most of these compounds are magnetic. Although antiferromagnetic order is most common, ferromagnetism is predicted in MSiSe₃ for M= Mn, Ni, in MSeTe₃ for M= V, Ni, in MnGeSe₃, in MGeTe₃ for M=Cr, Mn, Ni, in FeSnS₃, and in MnSnTe₃ for M= V, Mn, Fe. Among these compounds CrGeTe₃, VSnTe₃, CrSnTe₃ are ferromagnetic semiconductors. Our calculations suggest that the competition between antiferromagnetic and ferromagnetic order can be substantially altered by strain engineering, and in the semiconductor case also by gating. The associated critical temperatures can be enhanced by means of carrier doping and strains.

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I. INTRODUCTION

2D materials research has now broadened beyond graphene²⁵ to include other classes of van der Waals materials¹ including transition metal chalcogenides (TMC).⁴ These materials can be metals or semiconductors, have exceptionally strong light-matter coupling,⁵,⁶ and include ordered phases with charge density waves or superconductivity.⁵,⁶ Because of their potential importance for non-volatile information storage or logic device applications, the identification of two-dimensional (2D) materials with room-temperature magnetic order is an important research goal. Unfortunately single-layer magnetism has so far been realized only in relatively fragile 2D materials.¹⁰–¹⁵ Other van der Waals magnetism systems have so far been thinned only to several layers¹⁶–²⁰, or prepared only in bulk form.²¹–³⁷ No single-layer 2D materials have been discovered that exhibit room-temperature magnetism.

Magnetic 2D materials that have been proposed theoretically over the last few years include tritellurides based on chromium such as CrSiTe₃,³⁸–⁴³ and CrGeTe₃,⁴¹–⁴⁷, CrSnTe₃,⁴⁸ MPX₃ ternary chalcogenophosphates,⁵⁹–⁶⁵ and transition metal tri-³¹ and di-chalcogenides.⁵⁷–⁷⁸ The CrATe₃ (A= Si, Ge)⁴¹ ternary tritellurides have been predicted to be bulk ferromagnets with small bulk band gaps.π¹⁴ Temperature dependent transport¹⁴ and neutron scattering²² measurements are suggestive of 2D magnetism in these materials. Transition temperature Tₘ estimates are dependent on thickness, varying for example from 33 K for bulk CrSiTe₃,¹⁴ to 80 K in monolayers, and exhibiting the opposite behavior in CrGeTe₃ layered materials where Tₘ decreases in thinner layers because of weak magnetic anisotropy.¹⁶ Other non-chalcogenide transition metal magnetic layered materials like the tri-⁷⁹–⁸⁷ and di-halide⁸⁸–⁹² are expected to be ferromagnetic semiconductors with Curie temperatures typically below one hundred Kelvin. A recent breakthrough experiment has demonstrated CrI₃ devices in ultrathin layered form and revealed an intricate competition between ferromagnetic (FM) and antiferromagnetic (AFM) states as a function of layer number and external field.¹⁵

In this paper we present a DFT survey of the magnetic phases of MAX₃ single-layer transition metal trichalcogenide compounds covering a variety 3d transition metals (M= V, Cr, Mn, Fe, Co, Ni), the group IV elements (A= Si, Ge, Sn), and the three chalcogen atoms (X= S, Se, Te). These single-layer compounds are structurally closely related to their transition metal trichalcogenide MPX₃ cousins, which we studied in a recent related paper.⁴¹ The main difference between MAX₃ and MPX₃ compounds is that the group V phosphorus (P) atom inside the (P₂X₆)₃⁻ skeleton are replaced by (A₂X₆)₆⁻ bipyramids with group IV elements A = (Si, Ge, Sn). The change from P to A group IV element is responsible for important modifications in electronic and magnetic properties. We have examined the magnetic phase competitions between ferromagnetic (FM) and a variety antiferromagnetic (AFM) states, and the competition between magnetic and non-magnetic (NM) phases, as a function of electron carrier density and strain. While density functional theory does not always reliably capture the correlations present in transition metal compounds, we expect that our study, which is carried out under a unified framework, should provide useful insight into property trends in this class of materials.

Our paper is structured as follows. In Sec. II we summarize the technical details of our first principles electronic structure calculations. In Sec. III we discuss results for ground-state properties including structure, magnetic properties, and electronic band structures and densities-of-states. In Sec. IV we analyze the carrier-density dependence and the influence of strain on the magnetic phase competition. Finally in Sec. V
we close the paper with the summary and discussions.

![Diagram of MAX$_3$ compounds](image)

**FIG. 1:** (Color online) Schematic representation of the atomic structure of MAX$_3$ compounds. (a) Atomic structure of a MAX$_3$ monolayer identifying two possible choices for the unit cells, a rectangular cell identified by red lines containing four transition metal atoms (M), and a smaller triangular cell identified by black dashed lines containing two transition metal atoms (M). (b) Side view and top view of single layer MAX$_3$ compound. The MAX$_3$ compounds have one fewer occupied band than MPX$_3$ compounds because of the replacement of P atom pairs by group IV atoms (A) pairs that have with one fewer valence electron. The M atoms form hexagons (light green lines) centered by the A (= Si, Ge, Sn) bright blue atoms which are in turn surrounded two pairs of chalcogen X (= S, Se, Te) triangles represented in orange. (c) Schematic illustration of the octahedral ligands that give rise to lower energy $t_{2g}$ and higher energy $e_g$ metal atom d orbitals. The $t_{2g}$ and $e_g$ degeneracies are lifted by lattice distortions, for example as illustrated by z-axis elongation of the octahedron.

II. *AB INITIO* CALCULATION DETAILS

The calculations described in this paper were carried out using the plane-wave DFT software Quantum Espresso$^{93}$ to obtain ground-state electronic structure using ultrasoft pseudopotentials (RRKJUS) for the semi-local PBE-GGA.$^{94}$ We have in addition added vdW-D2$^{95}$ corrections to perform GGA+D2 (hereafter referred to as DFT-D2) calculations as a reference calculation thought to provide a description of the in-plane covalent bonds that is improved relative to the LDA,$^{96}$ and to add a weak interlayer binding correction through the D2 contribution.$^{97}$ We have also corrected onsite repulsion by performing GGA+D2+U calculations (hereafter referred to as DFT-D2+U), normally assuming the value U=4 eV. In a few select cases involving Co and Ni metals we have used larger values of U in order to obtain ground states that are magnetic. In all cases the atomic structure has been optimized by relaxing forces below $10^{-5}$ Ry/a.u., while the total energy tolerance for the self-consistency was set to $10^{-10}$ Ry. The k-point sampling density used a regularly spaced $4\times4\times1$ k-point grid and the plane wave cut-off energy was set to 60 Ry. Out-of-plane supercell periods of 25 Å allowed for a vacuum spacing in excess of 15 Å between facing chalcogen atoms, making overlaps between the electron clouds associated with different layers negligible.

III. STRUCTURAL AND MAGNETIC PROPERTIES

The MAX$_3$ transition metal trichalcogenide layers consist of 3d transition metals M= (V, Cr, Mn, Fe, Co, Ni) anchored by ($A_2X_6$)$^{6−}$ bipyramid ions with X = (S, Se, Te) and A = (Si, Ge, Sn). The 12 electrons taken by the six chalcogen atoms per unit cell are partly compensated by the 6 electrons needed by sp$^3$ bonds with bridge A atoms, leaving a final 6$−$ valence state for the anionic enclosure. The triangular lattice of bipyramids provides enclosures for the transition metal atoms, forming a structure that is practically identical to that of MPX$_3$ compounds enclosed by ($P_2X_6$)$^{4−}$ bipyramids. The octahedral arrangement of the chalcogens surrounding the metal ions is expected to give rise to crystal or ligand exchange fields$^{98}$ that split the d-orbitals into triply degenerate $t_{2g}$ and doubly degenerate $e_g$ levels which can further split in the presence of distortions as illustrated schematically in Fig. 1. The main difference between MAX$_3$ and MPX$_3$ compounds is that the A atoms have one fewer electron compared to P atoms yielding compounds with larger nominal metal cation valences, $3^+$ in MAX$_3$ compounds vs. $2^+$ in the MPX$_3$ compounds. The magnetic moments are carried largely by the metal ions, but the interactions between moments is dependent on their hybridizations with both the chalcogens and the A bridge atoms. All the 2D MAX$_3$ crystals we considered are magnetically ordered within DFT-D2, except for CoAX$_3$, NiGeS$_3$ and NiSnX$_3$. These become magnetic only within DFT-D2+U and only for a sufficiently large onsite repulsion parameter. Fig. 2 summarizes the overall trends in magnetic condensation energy, *i.e.* in the energy gained by forming a magnetically ordered states. These results show a strong tendency for magnetism for Cr compounds in which the $t_{2g}$ bands are close to half-filling, and weak in Co compounds in which the $t_{2g}$ bands are filled. It is clear therefore that crystal field effects play a strong role in the magnetism of these compounds. In the following we present an analysis of the structural, magnetic and electronic properties of representative 2D transition metal MAX$_3$ trichalcogenides, emphasizing their dependence on the chalcogen element (Si, Ge, Sn) and their underlying
electronic band structures.

FIG. 2: (Color online) Magnetic condensation energy trends. The energy gained per metal atom due to magnetic order obtained within DFT-D2 and DFT-D2+U (≈ 4 eV). In the cases of CoATE_3, CoASE_3 (A = Ge, Sn), and CoSnS_3 we choose the U parameter values of 5, 6, and 7 eV respectively in order to obtain a magnetic ground-state. Energy differences are not shown for cases in which metastable magnetic solutions could not be obtained.

A. Atomic structure of the lattice

The atomic structure in the single layer limit have been obtained by relaxing the structures using rectangular unit cells defined by two perpendicular vectors that we label with a and b, see Fig. 1, and an additional layer thickness c′ parameter defined as the distance between the chalcogen atom planes of the same MAX_3 single layer sandwiching the metal ions. The relaxed structures both for in-plane lattice constants and layer thickness of the rectangular unit cells, as obtained using DFT-D2 (See Supplemental Material as Fig.S1 and Table.I), are found to increase for larger chalcogen atoms for given A (Si, Ge and Sn) atoms. In general the calculated self-consistent lattice constants depend on the magnetic ordering. The variation is substantial for the transition metals V, Cr, Mn, Fe for all combinations of A (Si, Ge, Sn) and chalcogens S, Se, Te, up to 10% for in-plane lattice constants and up to 20% for the layer thickness, see Fig. 3. For compounds with Co and Ni the lattice distortions are much smaller. As a rule of thumb we can see that the magnitude in the distortion of the bonds is roughly proportional to the total energy differences represented in Fig. 2 and therefore they are largest when we compare magnetic and non-magnetic phases. The negative and positive values represent respectively compression and expansion during this non-magnetic to magnetic transition. The upper panel data a) represent calculations within DFT-D2 and the lower panel b) within DFT-D2+U. The latter shows generally greater variations in the lattice constants.

FIG. 3: (Color online) Relative distortion of the lattice parameter for different magnetic phases FM, nAFM, zAFM and sAFM measured with respect to the structural parameters obtained for non-magnetic phases using a rectangular unit cell with in-plane lattice parameters a(Å) and b(Å), and layer thickness c′(Å). The negative and positive values represent respectively compression and expansion during this non-magnetic to magnetic transition. The upper panel data a) represent calculations within DFT-D2 and the lower panel b) within DFT-D2+U. The latter shows generally greater variations in the lattice constants.

B. Magnetic configurations

The magnetic ground-state and meta-stable magnetic configurations are obtained by identifying energy extrema via

energy differences between magnetic and non-magnetic phases that are roughly doubled (see Fig. 2) within DFT-D2+U when compared to DFT-D2, and this difference is reflected in the increase of the lattice distortions. The relative difference of the lattice parameters between DFT-D2-U and DFT-D2 geometries are comparable to the difference between magnetic and non-magnetic phases within the same DFT approximation, see Fig. 3, and the Fig. S1 in the Supplemental Materials. This observation indicates that the short-range correlations of the transition metal atoms will generally impact the ground-state magnetic properties.

The magnetic ground-state and meta-stable magnetic configurations are obtained by identifying energy extrema via
converged self-consistency using initial conditions corresponding to Néel antiferromagnetic (nAFM), zigzag antiferromagnetic (zAFM), stripy antiferromagnetic (sAFM), ferromagnetic (FM), and nonmagnetic (NM) states. The analysis of the magnetic ground states obtained for the single layer MAX$_3$ compounds indicate that the magnetic moments are usually concentrated mostly at the metal atoms for AFM phases, a fact that simplifies our analysis of the magnetic solutions based on effective models. However, when the magnetic configuration is ferromagnetic we observe that a non-negligible spin polarization develop at the group IV and chalcogen atom sites of 0.3 $\sim$ 0.8$\mu_B$ in CrSiX$_3$. The specific magnetic solution will depend on the orbital hybridization between the metal ion and surrounding atoms to either suppress or enhance the tendency of the 3d transition metal elements to order magnetically. As discussed earlier, the transition metal atoms in 2D MAX$_3$ crystals can be viewed as contained in bipyramidal molecular cages formed by group IV A (Si, Ge, Sn) atoms and chalcogens that interact with the metal atoms. The relatively weak hybridization between the neighboring transition metal atom orbitals indicate that the inter-metal exchange interactions is mediated indirectly through the intermediate atoms. We have estimated the exchange interactions from ab initio electronic structure calculations from the total energies corresponding to antiferromagnetic, ferromagnetic, and nonmagnetic phases, see Fig. 2. In Table I of the Supplemental Material as Table-II and III$^{99}$ we present the numerical values for the total energies corresponding to the different magnetic configurations. Our results indicate that the magnetic phases are normally favored over the nonmagnetic solutions. Exceptions to this rule are the non-magnetic phases predicted within DFT-D2 for CoAX$_3$, NiGeS$_3$ and NiSnX$_3$. These compounds do develop magnetic solutions when we use a sufficiently large onsite repulsion parameter U within DFT-D2+U. We have generally used the $U=4$ eV value to assess the role of onsite Coulomb repulsion on the magnetic ground state energies, and used larger values ($U=5$ eV for CoGeTe$_3$, CoSnTe$_3$, $U=6$ eV for CoGeSe$_3$, CoSnSe$_3$, and $U=7$ eV for CoSnS$_3$) to obtain magnetic solutions when they did not appear for $U=4$ eV. Our DFT calculations predict that the Ni based trichalcogenides are magnetic only for some of the considered spin configurations. For instance NiGeS$_3$ and NiSnX$_3$ are non-magnetic within DFT-D2, and zAFM and sAFM phases are missing in NiSiS$_3$ and NiGeS$_3$, and NiGeTe$_3$ has only ferromagnetic ordering. Within DFT-D2+U it is possible to obtain both FM and nAFM for NiGeTe$_3$, and FM only for NiSnTe$_3$.

By considering that the magnetic moments are almost entirely located at the metal atoms in a honeycomb array we write the total energies per metal atom using an effective classical spin Hamiltonian as follows:

$$H = -\sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j - \frac{1}{2} \sum_{i\ne j} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

(1)

where the coefficients $J_{ij}$ represent the exchange coupling between two metal atom sites, the $\vec{S}_i$ represents the spin magnetic moment at the metal atom site labeled by $i$. We take semi-integer values $S = M/\mu_B$ for spin magnitudes, where $M$ represents the magnetic moments per metal atom for single layer magnetic MAX$_3$ structures and $g = 2$. This notation convention is different from a previous work on MPX$_3^{34}$ resulting in $J$ parameters that are four times larger and have reversed sign. The double-counting of the interactions are corrected by the 1/2 prefactor in Eq. 1. From the total energies for a unit cell with four metal atoms corresponding to ferromagnetic (FM), Néel (nAFM), zigzag AFM (zAFM), and stripy AFM (sAFM) configurations shown in Fig. 4.$^{99,100}$ and assuming a relatively short ranged magnetic interactions consisting of three $J_1$, $J_2$, $J_3$ parameters we can obtain:

$$E_{FM} - E_{AFM} = 3(J_1 + J_3) \vec{S}_A \cdot \vec{S}_B$$

(2)

$$E_{2AFM} - E_{zAFM} = (J_1 - 3J_3) \vec{S}_A \cdot \vec{S}_B$$

(3)

$$E_{FM} + E_{AFM} - E_{2AFM} - E_{zAFM} = 8J_2 \vec{S}_A \cdot \vec{S}_B,$$

(4)

where in the above equations we used the spin vectors $\vec{S}_A/B$ in dimensionless units acting on the triangular sublattices A and B in a honeycomb lattice. The average magnetic moments in units of $\mu_B$ calculated within DFT-D2 and DFT-D2+U are presented in Table I. The list of $J$ parameters for all the MAX$_3$ compounds are in Table II. We notice that for MAX$_3$ compounds where A=Si we get numerical values for the magnetization at V, Cr, Mn, Fe sites close to 2, 3, 4, 1 $\mu_B$ while for A=Ge, Sn we get 2, 3, 3, 1. Counting the number of 3d electrons filling of the $t_{2g}$ and $e_g$ bands we can make sense of the total magnetization dependence on the number of valence electrons. We note that the atomic 4s levels of the transition metal atoms in the $3^+$ cations lie higher up in energy than the

**FIG. 4**: (Color online) Schematic representations of different magnetic configurations in a honeycomb lattice of transition metal atoms where the magnetic moments are primarily located. We can classify the phases as (a) ferromagnetic, (b) Néel antiferromagnetic, (c) zigzag antiferromagnetic and (d) stripy antiferromagnetic. The exchange coupling constants $J_1$, $J_2$, and $J_3$ represent respectively the first, second, and third nearest neighbors of the central atom site that are indicated by the green (short dashes), the orange (dash-dotted), and navy blue (dashed) lines.
FIG. 5: (Color online) DFT-D2 band structures for single-layer MAX$_3$ compounds in their lowest-energy magnetic configurations for M = V, Cr, Mn, Fe, Co and Ni transition-metal atoms combined with A = Si, Ge, Sn group IV and X = S, Se, Te chalcogen atoms. The plotted band structures were calculated using the triangular structural unit cell, except for the cases of sAFM and zAFM that have a larger periodicity in the magnetic structure. There we used a triangular unit cell with doubled lattice constant. The bands are violet for AFM configurations, violet and orange for the up and down split spin bands in the FM configurations, and green for the NM phases. The Fermi energy is positioned at $E = 0$.

3d levels and they can be ignored. For example in the case of the vanadium atom with five valence electrons, two from 4s and three from 3d atomic orbitals, it is finally left with two unpaired 3d electrons leading to $2\mu_B$ in the $3^+$ cation configuration. Following this reasoning the magnetization increases as we move to the right in the periodic table until it reaches a maximum for Mn$^{3+}$ with four Bohr magnetons. The drop in magnetization to one Bohr magneton for Fe$^{3+}$ may be attributed to changes in the level ordering such that the five 3d electrons arrange into three and two electrons with opposing
FIG. 6: (Color online) The DFT-D2 density of states (DOS) for single-layer MAX$_3$ compounds in their lowest-energy magnetic configurations for M = V, Cr, Mn, Fe, Co and Ni transition-metal atoms with combination of A = Si, Ge, Sn and X = S, Se, Te chalcogen atoms. Different colors, gray for AFM configurations, red for states in the FM configurations, and green for the NM phases are used to facilitate the classification of the expected magnetic phases. Most ferromagnetic solutions are metallic except for VSnTe$_3$ and CrGeTe$_3$, while both gapped and metallic antiferromagnetic phases are common. The Fermi energy is positioned at $E = 0$. 
spin alignments. If crystal field splitting is large we should expect strongest magnetism when the $\varepsilon_{g}$ levels are half-filled or when the $\varepsilon_{u}$ levels are half filled i.e. around $d^{3}$ and $d^{6}$. For example for $3^{+}$ cations Cr is in $d^{3}$ state exhibiting magnetism, whereas Co in $d^{6}$ is expected to have its magnetism suppressed when crystal field effects are strong. The small departures in the numerical magnetic moments from the integer values may be attributed to the metallicity of the electronic structure that allows for non-integer magnetic moments and to the partial hybridization of the $d$ electrons of the transition metals with the surrounding chalcogens and bridge A atoms which makes the crystal-field interpretation for the transition metal bands less accurate.

The critical Néel or Curie temperatures $T_{c}$ for magnetic ordering were obtained from the diverging point of the heat capacity $C = (\langle E^2 \rangle - \langle E \rangle^2) / (kT^2)$ versus temperature, where $k$ is the Boltzmann constant. We have used the Metropolis Monte Carlo simulations of Ising models in periodic lattices of up to $50 \times 50$ sites in size. Numerical results for the heat capacity as a function of temperature that we used to extract the critical temperatures are presented in the Supplemental Material as Fig.S17. The critical temperatures $T_{c}$ of the Ising model listed in Table II should be considered upper bounds for the Heisenberg Hamiltonians when their anisotropy energy is very large. Therefore, it is expected that the actual critical temperatures are generally substantially smaller.

We have further compared our results against the anisotropic Heisenberg model whose total energy per metal atom reads

$$H = -\frac{1}{2N_{\text{cell}}} \sum_{i,j} J_{ij} \left( S_{i}^{x} S_{j}^{x} + S_{i}^{y} S_{j}^{y} + S_{i}^{z} S_{j}^{z} \right) + E_{\text{ani}}(\theta)$$

(5)

where $E_{\text{ani}}(\theta)$ is the total energy difference between the easy axis to all possible spin directions $\theta$ where $N_{\text{cell}}$ is the total number of metal atoms in the supercell. We assumed $E_{\text{ani}}(\theta, \phi) \approx E_{\text{ani}}(\theta)$ neglecting the weak $\phi$ dependence in the $x - y$ plane. The scan of total energies for all spin directions is done by performing calculations based on fully-relativistic pseudopotentials on top of atomic coordinates obtained relaxing with scalar relativistic pseudopotentials. We define the magnetocrystalline anisotropy energy (MAE) as the difference of total energy between two spin directions calculated for the easy and hard axes

$$\text{MAE} = \max \left( E_{\text{ani}}(\theta) \right)$$

(6)

that by definition will be a positive number. We list in Table I the magnetic anisotropy energies (MAE) calculated for the FM and nAFM phases. These energies are obtained by first relaxing the ground states within scalar-relativistic spin collinear calculations, and then orienting the spin directions within the fully-relativistic spin non-collinear calculations. The $E_{\text{ani}}(\theta)$ can be fitted by

$$E_{\text{ani}}(\theta) \simeq \sum_{n=0}^{N} a_n \cos(n\omega \theta) + \sum_{n=0}^{N} b_n \sin(n\omega \theta)$$

(7)

where the fitting coefficients ($a_n, b_n$) are listed in the supplemental material as Tables V and VI. An excellent fit is obtained using a few terms in the expansion although in certain cases we have used up to $N = 8$ for an accurate fit. The plots for the $E_{\text{ani}}(\theta)$ is presented in the supplemental material in Figs. S15 and S16.

The calculated average values of the magnetic moments at the metal sites vary widely depending on which metal atom we are considering, whereas the numerical averages of the magnetic moments for different magnetic configurations of the same compound have usually smaller differences (between $3\% \sim 10\%$), see Table I. The extracted critical temperatures $T_{c}$ of Heisenberg model listed in Table II, and the heat capacity plots are presented in the Supplemental Material as Fig. S18. The Heisenberg Monte Carlo calculations follow a recipe outlined in Ref. [103] and explained in Refs. [104,105] The lattice sites with $50 \times 50$ with brick lattice configurations used to perform the Monte Carlo calculations in honeycomb lattice in both the Ising and Heisenberg calculations. Total 200000 Monte Carlo steps were used, among them 100000 step for each thermalization and for averaging the observables.

### C. Electronic structure and density of states

We now turn our attention to the electronic band structure and density of states that dictate the electronic properties of these materials. In particular it is desirable to understand the interdependence between electronic structure and the magnetic configuration to explore applications that couple the spin and charge degrees of freedom in transport or optical experiments. The electronic structure of MAX$_{3}$ materials were obtained within DFT+D2 and DFT+D2+U, and among the materials studied there are both ferromagnets and antiferromagnets, and both metals and insulators. See Table III for a list of the different solutions. We have loosely classified as semimetallic those states with vanishingly small gaps or small density of states (DOS) near the Fermi energy from inspection of the electronic structure. The electronic band structures for the ground state configurations are shown in Fig. 5, and the corresponding DOS can be found in Fig. 6 for DFT-D2 (see Supplemental material for band structures and the corresponding DOS for DFT-D2+U as Fig.S2 and S3).

The band structure plots have used a triangular unit cell around one of the $K$ valleys, while we doubled the cell size to allow for longer period zAFM and sAFM magnetic configurations. The DOS for all magnetic (FM, nAFM, zAFM and sAFM) and non-magnetic phases within DFT-D2 and DFT-D2+U as well as the analysis of the orbital projected partial density of states in the Supplemental Material as Fig.S4 and S5 reveals that the conduction or valence band edges have an important contribution from the $d$ orbitals of metal atoms as well as $s$ and $p$ orbitals of the A, X atoms.

The k-point resolved orbital projected density of states for the specific case of CrGeTe$_{3}$ shown in Fig. 7 allows to visualize the orbital contributions from all three atoms and the degree of their hybridization for the states near the valence and conduction band edges. The differences in the density
of state profiles between DFT+D2 and DFT+D2+U calculations indicate that the electronic structures depend sensitively on the choice of electron-electron interaction model which tend to split further the d-orbital bands. As expected, most

interfaces when the electrons at the band edge are predominantly distributed at the chalcogens.

IV. CARRIER AND STRAIN TUNABLE MAGNETISM

As we reported in the case of MPX$_3$ layered compounds the possibility of altering the properties of 2D magnetic materials by means of externally tunable parameters make these materials promising for a host of spintronics applications. The main two control knobs that we explore in this section are the carrier density and strains. Carrier density doping can be envisioned through field effects in transistor setups or by forming interfaces with charge polarized ferroelectric materials or ionic molecules. If magnetic transitions can be achieved with carrier densities accessible in conventional transistors they would provide a convenient route for electrical manipulation of magnetic properties. Likewise, the strains generated by mechanical bending, pressure or stretching of 2D materials would pave the way towards piezomagnetic control.

A. Field-effect control of magnetic properties

The possibility of controlling the magnetic properties of a device through a gate voltage offers advantages over magnetic-field mediated control in terms of speed and spatial resolution. If achieved using 2D material devices they would have an additional advantage of further reduced energy cost per device operation compared to conventional devices. Control of magnetic order through electric fields have been achieved in ferromagnetic semiconductors and in metal films where the magnetic exchange coupling and the magnetic anisotropy can be tuned by modifying the position of the Fermi level. A schematic illustration for a field effect transistor device where magnetic order is modified through a carrier inducing backgate is shown in Fig. 8 for DFT-D2 (see Supplemental material for using DFT-D2+U method as Fig.S12). In this same figure we summarize our results for the theoretically predicted trends for the competition between AFM and FM states for 2D MAX$_3$ compounds that we have considered. In our calculations we have obtained the variation of the total energy differences between magnetic configurations as a function of carrier density neglecting the effects of carrier inhomogeneity within the layer due to the presence of external electric fields. When the ground state is in the AFM phase it is often possible to trigger a transition to FM phases. Field-effect mediated control in terms of speed and spatial resolution. If achieved using 2D material devices they would provide a convenient route for electrical manipulation of magnetic properties. Likewise, the strains generated by mechanical bending, pressure or stretching of 2D materials would pave the way towards piezomagnetic control.

\[
\delta E(\pm \delta n) = \delta E_0 + (\Delta E_{\text{gap}} / 2 \pm \delta \mu)(\pm \delta n) \quad (8)
\]
FIG. 8: (Color online) Carrier density dependent total energy differences per MAX$_3$ formula unit between the AFM and FM phases of V, Cr, Mn, Fe, Ni based single layer trichalcogenides obtained within DFT-D2. The AFM ground-states favored near charge neutrality can often be switched to FM phases either for electron or hole doping for sufficiently large carrier densities in V, Mn, Ni, and Fe based compounds. Cusps in the total energy differences are seen near charge neutrality in gapped AFM materials manifesting the transition from electron to hole doping. Carrier densities of up to a few $\sim 10^{14}$ electrons per cm$^2$ should be in principle accessible through ionic liquid or gel gating. A carrier density of 0.1 electrons per MAX$_3$ formula unit corresponds to $\sim 6 \times 10^{13}$ electrons per cm$^2$ when the distance between the metal atoms is $\sim 6$Å.

We label within brackets the expected phase i.e., nonmagnetic (NM), Néel antiferromagnetic (nAFM), zigzag antiferromagnetic (zAFM) and stripy antiferromagnetic (sAFM) that transition from ferromagnetic (FM) state next to each compound.

where the carrier density of $n$-type samples is $+\delta n$, the density for $p$-type samples is $-\delta n$, the energy difference between AFM and FM phases in neutral MAX$_3$ sheets is given by $\delta E_0$, and the difference between the mid-gap energy in the AFM semiconductors and the chemical potential of the ferromagnetic phase is $\delta \mu$. Therefore, for positive (negative) $\delta \mu$ the transition from AFM to FM phase is most effective for electron doping (hole doping). We show in Fig. 9(a) the total DOS corresponding to FM and AFM phases of CrSiTe$_3$ in the presence of carrier doping as a specific example, while a detailed breakdown of the projected density of states at each atomic site as a function of carrier density can be found in the Supplemental Material as Fig.S13 and S14.$^{59}$ It is expected that the transition between AFM and FM phases can happen for relatively small total carrier density modification when the total energy difference per formula unit is smaller than the band gap. We can see in Fig. 8 that magnetic phase transitions are expected in CrSiTe$_3$, MnSiX$_3$, CrGeSe$_3$ at electron carrier densities and MnSiS$_3$, FeSiSe$_3$, FeGeSe$_3$, VSnSe$_3$ at hole densities as small as $\sim 0.05$ electrons per formula unit which correspond to carrier densities on the order of $\sim 10^{13}$cm$^{-2}$. Carrier densities of this magnitude could be achievable in field
FIG. 9: (Color online) The evolution of the three nearest neighbor exchange coupling J parameters as a function of (a) carrier doping per formula unit, and (b) bi-axial strain imposed by modifying the dimensions of the rectangular unit cell. (c) The variation of critical temperature as a function of carrier doping (top) and bi-axial (bottom) strain in CrSiTe$_3$ (left panel) and CrGeTe$_3$ (right panel), calculated within DFT-D2 and DFT-D2+U.

Ultrathin 2D-materials lie at the frontier between soft and hard condensed matter thanks to their membrane-like flexibility which has led to proposals that engineer their electronic properties by means of strains. Taking graphene as an example, the appropriate generation of strains could lead to large pseudomagnetic fields or cause the generation of primary Dirac point band gaps in nearly aligned graphene on hexagonal boron nitride. In order to assess the role of strains in the electronic structure of ultrathin 2D MAX$_3$ materials we calculate the total energies of the different magnetic phases in the presence of expansive or compressive in-plane biaxial strains that we model by uniformly scaling the rectangular unit cell, see Fig. 10. The uniform biaxial strains lead to modifications in the magnetic phase energy differences $E_{\text{AFM}} - E_{\text{FM}}$ that can trigger phase transitions for strains as small as 2-4% in certain cases, while much larger strain fields are required in general. In the following we list the five different types of strain-induced effects expected in charge neutral MAX$_3$ compounds:

- **No phase change (expansion and compression):** The ground-states are not altered in the presence of strains for vanadium based VSiS$_3$ (sAFM), VSiSe$_3$ (zAFM), chromium based CrSiS$_3$ (nAFM), CrSiSe$_3$ (nAFM), CrGeS$_3$ (nAFM), CrSnS$_3$ (zAFM), manganese based MnGeTe$_3$ (FM), iron based FeSnS$_3$ (FM), FeSnTe$_3$ (FM), and nickel based NiGeTe$_3$ (FM).

- **AFM to FM (compression):** For compressive strains we find transitions in vanadium based VSiSe$_3$ (∼4%), VGeS$_3$ (∼1%), VGeSe$_3$ (∼4%), VGeTe$_3$ (∼9%), chromium based CrSiTe$_3$ (∼1%), CrGeTe$_3$ (∼7%), manganese based MnSiS$_3$ (∼2%), MnSiTe$_3$ (∼1%), MnGeS$_3$ (∼1%), MnGeSe$_3$ (∼1%), MnGeTe$_3$ (∼1%), iron based FeSiS$_3$ (∼4%), FeGeS$_3$ (∼4%), and nickel based NiGeS$_3$ (∼4%).

- **FM to AFM (expansion):** Conversely for expansive strains we find transitions in vanadium based VGeS$_3$ (∼12%), VSnSe$_3$ (∼2%) chromium based CrSiTe$_3$ (∼2%), CrSnTe$_3$ (∼8%), manganese based MnSiTe$_3$ (∼6%), iron based FeSiSe$_3$ (∼1%), FeGeSe$_3$ (∼1%), FeSnTe$_3$ (∼4%) and, nickel based NiSiSe$_3$ (∼1%).

- **FM to AFM (compression):** Transitions are seen for compressive strains (%) in vanadium based VSiTe$_3$ (∼1%), VSnTe$_3$ (∼1%), chromium based CrGeTe$_3$ (∼2%), CrSnTe$_3$ (∼2%), iron based FeSiS$_3$ (1%) and, nickel based NiSiSe$_3$ (4%), NiSiTe$_3$ (4%).

- **FM to AFM (expansion):** Transitions for expansive strains (%) are found for manganese based MnSiSe$_3$ (∼1%), MnSnTe$_3$ (4%), iron based FeSiS$_3$ (4%), and nickel based NiSiSe$_3$ (4%), NiSiTe$_3$ (4%).

An example about the DOS evolution as a function of strain is shown in Fig. 9 (b) for charge neutral CrSiTe$_3$ monolayer subjected to ∼4% (compressive) and 4% (expansive) strains in the FM and zAFM phases. The expansion strains are found to have a small effect in both the FM and zAFM phases of CrSiTe$_3$ but compressive strains of 4% lead to a closure of the FM-CrSiTe$_3$ band gap turning it into a semi-metal with a small finite density of states at the Fermi level. As mentioned earlier, from the projected density of states analysis in the Supplemental Material as Fig. S13-S14 we can observe a relatively large content of Cr-$d$ and Si-$s$, $p$ orbitals at the bands near the Fermi energy.
FIG. 10: (Color online) Influence of in-plane strain on the magnetic configurations of selected MAX₃ compounds. Magnetic phase transitions are introduced by in-plane biaxial compressive and expansive strains for several magnetic MAX₃ compounds at zero carrier density. We notice that the magnetic phase energy differences in some compounds are especially susceptible to the strains suggesting that large variations in T_c values may be achievable by strain engineering. We indicate next to each chalcogen atom label the magnetic configuration to which the FM phase transitions.

The Fig. 9(c) illustrates how the T_c can be modified by carrier density variations or strains that can be applied in the system by gating or compression/expansion of the sample (see Supplemental material for J parameters comparison as function of strain and carrier doping as Table IV). For monolayer CrSiTe₃ we showed that substantial increases of the T_c can be achieved for large hole doping and compressive strains.

V. SUMMARY AND CONCLUSIONS

In this work we have presented an ab initio study for the electronic and magnetic properties of single layer MAX₃ transition metal trichalcogenide materials composed by 3d transition metal (M = V, Cr, Mn, Fe, Co, Ni), group IV elements (A = Si, Ge, Sn) and chalcogen (X = S, Se, Te) atoms. Our DFT calculations indicate that a variety of magnetic ground
states are supported depending on material composition, including AFM phases in either Néel, stripy, zigzag configurations, as well as FM configurations. The various magnetic phases including FM, AFM and non-magnetic (NM) phases are found to exist for both metallic and semiconducting states indicating the large pool of material combinations possible for prospective applications in devices. The specific choice of the unit cell either triangular or rectangular as well and the supercell dimension impact the total energy of the ground states for the different magnetic phases which indicates the sensitivity of the magnetic ground-state solutions to the geometry of the chemical bonds. Compounds such as CoAX$_3$ and NiAX$_3$ are non-magnetic within semi-local DFT-D2, although they can stabilize magnetic phases upon inclusion of a sufficiently large U at the metal atom sites. The important differences in the predicted results obtained within DFT-D2 and those obtained including a local U correction indicate the importance of correctly capturing the Coulomb correlation effects and calls for further experimental search of this class of material compounds to combine the results with the theoretical modeling of the exchange interactions. We have analyzed the stability of the magnetic phases on the Ising model of a honeycomb lattice where the exchange coupling parameters are obtained from the total energy differences corresponding to different meta-stable spin configurations. This approach is expected to be valid for insulating phases with localized electrons and when the magnetic anisotropies are large. The critical temperatures that we obtained within the same unified Metropolis statistical analysis framework$^{104}$ should be seen as an upper bound for the expected critical temperatures of a classical Heisenberg model with magnetic anisotropy. We have then obtained the magnetic phase diagram map as a function of carrier density and strains which should be parameters that are controllable in experiments. The devices based on 2D materials are particularly suited for field effect control of carrier density which can be enhanced by using high k-dielectrics, ionic liquids, or by interfacing with ferroelectric materials. We have also explored the possibility of modifying the magnetic phases by means of strains and found that the ground state magnetic configuration can undergo phase transitions driven by in-plane compression or expansion of the lattice constants as small as a few percents in certain cases. Our study suggests that the large variety of available material compositions of single layer MAX$_3$ transition metal dichalcogenides and the possibility of controlling environment parameters such as carrier density and strains in experiments makes these materials promising for 2D spintronics research. These control knobs can be useful not only for triggering magnetic phase transitions but for enhancing the critical temperatures of the magnetic phases to make the devices more useful in practical applications.

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See the Supplemental Material for the total energy difference, lattice constants, the J-Coupling parameters along with magnetic moments and transition temperatures using DFT-D2, band structures, the associated density of states and the orbital projected density of states (PDOS) calculated for self-consistently converged magnetic configurations, the carrier density dependent density-of-states calculated for self-consistently converged magnetic configurations, the associated density of states and the orbital projected density-of-states calculated for self-consistently converged magnetic configurations, the carrier density dependent density-of-states calculated for self-consistently converged magnetic configurations.

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|          | DFT-D    | DFT-D-U  |
|----------|----------|----------|
| MAX3     |          |          |
| VSlSe    | 1.683    | 1.483    |
| VSlSe    | 1.787    | 1.546    |
| VSlTe2   | 1.932    | 1.788    |
| CrSiSe   | 2.759    | 2.604    |
| CrTe2    | 2.773    | 2.701    |
| CrTe2    | 2.851    | 2.794    |
| MnSiSe   | 3.612    | 3.423    |
| MnSiTe2  | 3.661    | 3.629    |
| MnSiTe2  | 3.741    | 3.719    |
| FeSiSe   | 0.983    | 1.025    |
| FeSiTe2  | 1.608    | 1.149    |
| FeSiTe2  | 1.160    | 1.247    |
| CoSiSe   | -        | -        |
| CoSiTe2  | -        | -        |
| NiSiSe   | 0.699    | 0.573    |
| NiSiTe2  | 0.646    | 0.491    |
| VGeSe3   | 1.651    | 1.473    |
| VGeSe3   | 1.660    | 1.532    |
| VGeTe3   | 1.891    | 1.700    |
| CrGeSe3  | 2.675    | 2.597    |
| CrGeSe3  | 2.758    | 2.688    |
| CrGeSe3  | 3.078    | 2.774    |
| MnGeSe3  | 2.798    | 2.529    |
| MnGeSe3  | 2.980    | 2.879    |
| MnGeTe3  | 3.331    | 3.155    |
| FeGeSe3  | 0.966    | 1.013    |
| FeGeSe3  | 1.050    | 1.135    |
| FeGeTe3  | 1.141    | 1.230    |
| CoGeSe3  | -        | -        |
| CoGeSe3  | -        | -        |
| CoGeTe2  | -        | -        |
| NiGeSe3  | 0.499    | 0.518    |
| VSnSe3   | 1.576    | 1.302    |
| VSnSe3   | 1.619    | 1.414    |
| VSnTe3   | 1.602    | 1.466    |
| CrSnSe3  | 2.623    | 2.345    |
| CrSnSe3  | 2.692    | 2.622    |
| CrSnTe2  | 2.894    | 2.895    |
| MnSnSe3  | 2.799    | 2.392    |
| MnSnSe3  | 3.043    | 2.750    |
| MnSnTe3  | 3.260    | 3.003    |
| FeSnSe3  | 0.929    | 0.938    |
| FeSnSe3  | 0.991    | 1.014    |
| FeSnTe3  | 1.088    | 1.193    |
| CoSnSe3  | -        | -        |
| CoSnTe2  | -        | -        |
| NiSnSe3  | 0.755    | 0.666    |
| NiSnSe3  | 0.789    | 0.725    |

**TABLE I:** Magnetic moments in Bohr magneton $\mu_B$ per metal atom for single layer magnetic MAX$_3$ structures, magnetic anisotropy energy (MAE) as the total energy difference for spins in the easy and hard axes. In the cases of CoAX$_3$, CoAX$_3$ (A=Ge, Sn), and CoSnS$_3$ the U parameter values used are 5, 6 and 7 eV, respectively. We use the labels of FM for ferromagnetic, nAFM for Néel antiferromagnetic, zAFM for zigzag antiferromagnetic, and sAFM for stripy antiferromagnetic configurations. The *ab initio* calculations were performed within DFT-D2 and DFT-D2+U.
| Coupling Strengths | $J_1$ | $J_2$ | $J_3$ | $J_{c1}$ | $J_{c2}$ | $J_{c3}$ | $J_{c4}$ |
|-------------------|-----|-----|-----|-------|-------|-------|-------|
| $\text{MAX}_3$ | 1.562 | -15.24 | -11.02 | -3.256 | 37.1 | 75.6 | 1.890 |
| $\text{NiGeSe}_3$ | 1.643 | 13.76 | -3.704 | -4.924 | 31.1 | 121.6 | 2.523 |
| $\text{FeGeTe}_3$ | 1.871 | 28.44 | -1.468 | -1.272 | 84.4 | 321.2 | 2.786 |
| $\text{CrSiSe}_3$ | 2.654 | -13.97 | -1.448 | -0.800 | 45.0 | 46.4 | 3.161 |
| $\text{CoSiSe}_3$ | 2.750 | -6.788 | -1.116 | -0.964 | 92.3 | 160.1 | 3.415 |
| $\text{CoTeSi}_3$ | 2.938 | 3.576 | -1.000 | -0.104 | 5.1 | 27.3 | 3.728 |
| $\text{MnSiS}_3$ | 3.522 | -2.820 | -1.000 | -1.920 | 30.1 | 118.8 | 4.346 |
| $\text{VGeS}_3$ | 1.536 | -12.02 | -10.76 | -9.112 | 27.3 | 108.2 | 1.882 |
| $\text{CrGeS}_3$ | 2.626 | -7.104 | -1.296 | -0.884 | 39.9 | 130.0 | 3.130 |
| $\text{FeGeS}_3$ | 2.919 | 4.712 | -0.116 | 0.972 | 64.5 | 230.2 | 3.718 |
| $\text{MnGeS}_3$ | 2.642 | -6.276 | -0.032 | 1.780 | 13.4 | 63.1 | 4.281 |
| $\text{CoGeS}_3$ | 1.536 | -4.512 | -6.848 | -6.512 | 29.7 | 105.4 | 2.348 |
| $\text{CrSiS}_3$ | 2.716 | -1.156 | -1.032 | -0.660 | 5.5 | 18.1 | 3.405 |
| $\text{CoSiS}_3$ | 2.919 | 4.712 | -0.116 | 0.972 | 64.5 | 230.2 | 3.718 |
| $\text{NiSiS}_3$ | 2.289 | 2.400 | 0.536 | 1.320 | 71.4 | 239.1 | 4.210 |
| $\text{NiGeS}_3$ | 3.226 | 1.636 | 0.576 | 0.772 | 64.9 | 221.4 | 4.399 |
| $\text{MnSnS}_3$ | 1.098 | -6.124 | 0.580 | -6.612 | 29.7 | 96.5 | 3.540 |
| $\text{FeSnS}_3$ | 1.201 | -106.0 | 34.47 | 65.20 | 135.1 | 552.8 | 3.389 |
| $\text{CoSnS}_3$ | 1.424 | 14.77 | -15.54 | 1.908 | 24.6 | 77.9 | 1.849 |
| $\text{VSnS}_3$ | 1.513 | 18.66 | -9.336 | -1.884 | 20.8 | 95.1 | 2.012 |
| $\text{VSiS}_3$ | 1.854 | 57.10 | -8.336 | -5.668 | 15.7 | 140.6 | 2.793 |
| $\text{CrSnS}_3$ | 2.566 | 7.100 | -4.308 | -4.060 | 70.7 | 259.9 | 3.034 |
| $\text{CoSiS}_3$ | 2.687 | 8.748 | -3.956 | -3.548 | 66.2 | 262.7 | 3.301 |
| $\text{CoTeSi}_3$ | 2.887 | -4.924 | -6.668 | 16.20 | 255.8 | 901.0 | 3.805 |
| $\text{MnSnS}_3$ | 2.546 | -29.88 | 2.368 | 3.056 | 24.6 | 95.6 | 4.022 |
| $\text{NiSiS}_3$ | 3.934 | 10.37 | 2.824 | 94.86 | 165.2 | 354.7 | 3.599 |
| $\text{FeSnS}_3$ | 1.001 | 22.97 | -3.287 | 17.26 | 36.2 | 98.8 | 3.451 |
| $\text{CoSiS}_3$ | 1.141 | -1.308 | 29.14 | 3.868 | 36.2 | 457.7 | 3.050 |
| $\text{CoSiS}_3$ | - | - | - | - | - | - | - |
| $\text{CoSnS}_3$ | - | - | - | - | - | - | - |
| $\text{NiSnS}_3$ | - | - | - | - | - | - | - |
TABLE III: Band gaps and electronic property of MAX$_3$ compounds. The band gaps are listed in eV energy units and their values and the magnetic configuration depend substantially on the exchange-correlation approximation employed within DFT-D2 and DFT-D2+U (= 4 eV). For CoAT$_3$, CoAS$_3$ ($A$ = Ge,Sn), CoSn$_3$ the $U$ parameter values chosen are 5, 6 and 7 eV respectively. Different calculation methods have been indicated by I:DFT-D2 and II:DFT-D2+U. The ground states for selected method are represented in boldface type and blue color (M:Metal; SM:Semi-Metal; HM:Half-Metal). We distinguish the different magnetic configurations Nonmagnetic (NM), Ferromagnetic (FM), Néel antiferromagnetic (nAFM), zigzag antiferromagnetic (zAFM) and, stripy antiferromagnetic (sAFM).

| A     | Si  | Ge  | Sn  |
|-------|-----|-----|-----|
| MAX$_3$ Method | NM  | FM  | nAFM| zAFM| sAFM| NM  | FM  | nAFM| zAFM| sAFM| NM  | FM  | nAFM| zAFM| sAFM|
| VAS$_3$ I | M 0.217 0.347 | M 0.185 | M 0.277 0.350 | M 0.402 | M | M 0.233 0.368 | M 0.179 |
| II | 0.888 1.588 | 1.583 1.292 1.277 | 0.678 1.687 | 1.699 1.397 1.403 | 0.371 0.549 | 1.456 | 1.97 | 1.247 |
| VAS$_3$ I | M 0.333 1.635 | 0.246 | M 0.150 0.355 | 0.344 | M | M 0.239 0.428 | 0.108 M |
| II | 1.301 1.665 0.106 | 0.251 | 0.646 1.260 | 1.565 | 1.555 | 0.111 | 0.385 0.484 | 1.335 | 1.017 0.769 |
| VAS$_3$ I | M 0.350 | M | M 0.093 0.203 | M | M | 0.173 | M | M |
| II | 0.708 | HM | M | M | M | 0.468 | M | M | M |
| CrAS$_3$ I | 0.038 1.221 | 1.602 1.082 | 1.001 | 0.103 | 1.169 | 1.456 | 0.947 | 0.974 | M | 0.598 0.855 | 1.74 0.757 |
| II | 0.273 0.989 | 1.226 | 0.865 0.701 | 0.074 | 1.069 | 1.313 | 1.311 | 0.793 | M | 0.550 0.861 | 1.047 0.950 |
| CrAS$_3$ I | M 1.066 | 1.234 | 1.010 | 0.839 | 0.021 | 0.879 | 1.135 | 1.115 | 0.703 | M | 0.674 0.941 | 0.823 0.406 |
| II | 0.157 0.536 | 0.890 | 0.937 | 0.454 | 0.181 | 0.531 | 0.799 | 0.859 | 0.427 | M | 0.316 0.470 | 0.654 | 0.505 0.432 |
| CrAT$_3$ I | M 0.645 0.776 | 0.378 | 0.817 | 0.118 | 0.421 | 0.705 | 0.432 | 0.270 | M | 0.527 0.545 | M |
| II | 0.155 0.455 | 0.624 | 0.106 | 0.034 | 0.169 | 0.529 | M | M | 0.112 0.178 | 0.365 M |
| MnAS$_3$ I | M 1.206 | HM | SM | 0.372 | M | M | M | 0.101 | M | M | M | M | 0.014 M |
| II | 0.229 | HM | M | M | M | 0.233 | HM | M | M | M | M | M | M | M |
| MnAS$_3$ I | M 0.101 | 0.082 | M | M | M | M | 0.101 | M | M | M | M | M | M | M |
| II | 1.206 | HM | SM | 0.372 | M | 0.101 | M | M | M | M | M | M | M | M |
| MnAT$_3$ I | M 0.591 | 0.729 | M | 0.099 | 1.028 | 0.129 | 0.785 | 0.730 | M | M | 0.487 0.510 |
| II | 0.016 | 0.716 | 0.569 | 0.730 | 0.089 | M | 1.242 | HM | M | M | M | M | M | M |
| FeAS$_3$ I | 0.298 | M | 0.703 | 0.514 | 0.180 | HM | M | 0.622 | 0.486 | M | M | 0.433 0.406 |
| II | 0.717 | HM | 0.455 | 0.655 | 0.605 | M | 0.391 | 0.567 | M | M | 0.982 M | M |
| FeAT$_3$ I | 0.080 0.642 | M | 0.487 | 0.378 | 0.069 | M | M | 0.533 | 0.310 | M | M | 0.208 0.101 |
| II | 0.487 | HM | 0.333 | M | M | 0.351 | M | 0.166 | M | M | M | M | M | M |
| CoAS$_3$ I | 0.899 | - | - | - | - | M | - | - | - | - | M | - | - | - | - |
| II | 1.259 | 1.259 | 0.428 | M | M | 1.061 | 1.060 | M | M | 0.302 | HM | 1.014 | 0.505 M |
| CoAT$_3$ I | 0.865 | - | - | - | - | M | 0.722 | - | - | - | - | M | 0.167 | - | - |
| II | 0.878 | 0.472 | 0.683 | 0.110 | M | 0.770 | 0.599 | 0.770 | 0.306 | 0.110 | M | 0.466 | M | 0.417 | 0.466 0.101 |
| CoAT$_3$ I | 0.550 | - | - | - | - | M | 0.383 | - | - | - | - | M | 0.172 | - | - |
| II | 0.552 | 0.555 | 0.555 | 0.211 | M | 0.404 | 0.409 | 0.299 | 0.165 | M | 0.246 | M | 0.246 M | M |
| NiAS$_3$ I | M 0.032 | SM | M | M | M | M | M | M | M | M | M | M | M | M | M |
| II | 0.032 | SM | M | M | M | M | M | M | M | M | M | M | M | M | M |
| NiAT$_3$ I | M | M | M | M | M | M | M | M | M | M | M | M | M | M | M |
| II | M | M | M | M | M | M | M | M | M | M | M | M | M | M | M |