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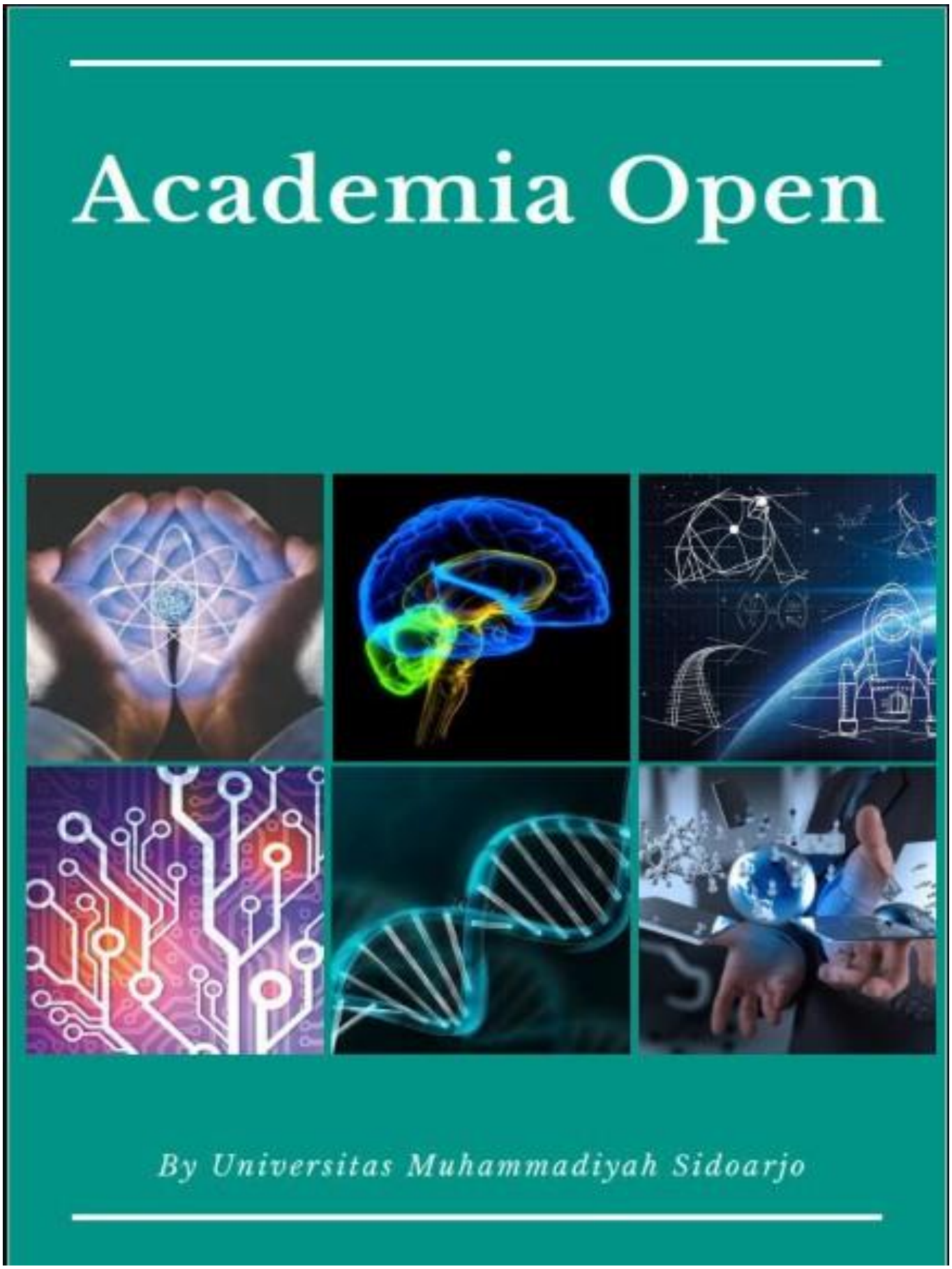
Vol. 11 No. 1 (2026): June
DOI: 10.21070/acopen.11.2026.14499



ISSN 2714-7444 (online), https://acopen.umsida.ac.id, published by Universitas Muhammadiyah Sidoarjo

Academia Open

Vol. 11 No. 1 (2026): June
DOI: 10.21070/acopen.11.2026.14499

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DOI: 10.21070/acopen.11.2026.14499

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Academia Open
Vol. 11 No. 1 (2026): June
DOI: 10.21070/acopen.11.2026.14499

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Academia Open

Vol. 11 No. 1 (2026): June
DOI: 10.21070/acopen.11.2026.14499

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Academia Open

Vol. 11 No. 1 (2026): June
DOI: 10.21070/acopen.11.2026.14499

Computational Study of Quantum Phases in 2D Magnetic Monolayers Under Strain and Doping

Doaa Ayad Kamil, doaaayad@uos.edu.iq (*)

Department of Science, Branch Physics College of Basic Education University of Sumer-Dhi Qar, Iraq

(*) Corresponding author

Abstract

General Background: Two-dimensional magnetic materials are promising quantum systems for studying electronic structure, magnetic ordering, and thermal stability in low-dimensional platforms. **Specific Background:** Materials such as CrI_3 and $Cr_2Ge_2Te_6$ exhibit intrinsic ferromagnetism that can be tuned through mechanical strain and electron doping. **Knowledge Gap:** Previous studies mainly examined strain and doping separately, with limited integrated analysis of their combined role in magnetic phase stability. **Aims:** This study investigates quantum phases in two-dimensional magnetic monolayers using density functional theory, XXZ-Heisenberg modeling, and Monte Carlo simulations under strain and electron doping conditions. **Results:** CrI_3 maintains intrinsic ferromagnetism with an out-of-plane easy axis and a Curie temperature of 45 K, while 5% compressive strain increases magnetic anisotropy energy by approximately 47%. Electron doping in $Cr_2Ge_2Te_6$ increases the exchange constant from 6.874 meV to 10.202 meV and raises the Curie temperature from approximately 85 K to 123 K at 0.3 e/cell. **Novelty:** The study integrates electronic structure, magnetic anisotropy, exchange interactions, and thermal behavior within a unified computational framework. **Implications:** The findings provide theoretical guidance for developing thermally stable two-dimensional magnetic materials for spintronics and quantum devices.

Highlights:

- CrI_3 monolayers preserve intrinsic ferromagnetism with out-of-plane magnetic ordering at 45 K.
- Compressive biaxial deformation increases magnetic anisotropy energy and stabilizes thermal magnetic behavior.
- Electron carrier injection in $Cr_2Ge_2Te_6$ raises exchange coupling and Curie temperature to 123 K.

Keywords: Two-Dimensional Magnetic Materials, Quantum Phases, Density Functional Theory, Electron Doping; Monte Carlo Simulation

Published date: 2026-05-28

Academia Open
Vol. 11 No. 1 (2026): June
DOI: 10.21070/acopen.11.2026.14499

Introduction

Two-dimensional magnetic materials have recently emerged as a hot topic in condensed matter physics. This allows its experimental investigation of electronic structure, magnetic order, along with thermal gradients in the lowest dimensional frameworks. The interest in the field soon arose with the experimental observation and its interpretation on intrinsic magnetism at the single-layer boundary of van der Waals crystals like CrI_3, cementing two-dimensional magnetism as a tunable and functionally important class of quantum materials (Algarni, M., et al. 2025; Liu, P., et al., 2023).

From these materials, the fact is that their magnetic behaviour is ruled by not only exchange but also magnetic anisotropy, spin-orbit coupling and electronics near the Fermi level. In 2D systems magnetic anisotropy is responsible for maintaining long range magnetic order at finite temperatures. Therefore, changes in crystal or electronic geometry are capable of modulating the magnetic phases and thermal stability (Algarni, M., et al. 2025; Kong, et al., 2024).

Two parameters that have received particular attention in tuning are mechanical stress and electron doping. Stress affects bond lengths and angles, orbital hybridization and magnetic anisotropy energy; and electron doping affects the charge carrier concentrations and exchange behaviors between the magnetic sites. Several previous experimental and computational investigations have reported that both parameters can significantly change the magnetic stability and Curie temperature of a two-dimensional magnet (Li, L., & Fyta, M. 2025; Hendriks, M., et al. 2025; Hu et al., 2023).

Methodologically, density functional theory offers a dependable, and theoretically sound, basis for describing ground state electronic and magnetic properties, and Monte Carlo simulation is suitable for studying thermal phenomena and magnetic phase transitions. Exchange coefficients and density functional theory-based magnetic anisotropy and state of the art efficient spin models have been shown to accomplish an exemplary combination in the characterization of fast-emerging 2D magnets (Bosoni, E., et al., 2024; Zhang, & Phanish, 2025; Kong, et al., 2024).

Although developments in this area have been rapid, there are few studies that successfully combine stress and charge doping on electronic behavior, magnetic anisotropy, exchange interactions, and thermal stability. Hence, here, we address the development of quantum phases in 2D magnetic monolayers under the combination of mechanical stress and electron doping by merging an approach combined with an integrated computational approach with an emphasis on density functional theory (DFT) and Monte Carlo simulation methods. This approach is anticipated to enhance our understanding of phase architecture in low-dimensional magnets and pave the way for spin-electronics and functional quantum materials applications (Mi, M.,2023; Zhang et al., 2024).

Research Problem

The main problem of this study is to determine how mechanical stress and electron doping affect the quantum phases emerging in two-dimensional magnetic layers, and how these changes influence their physical properties and technological potential (Algarni, M., et al. 2025; Li, L., & Fyta, M. 2025; Kong, et al., 2024; Hu et al., 2023).

Relevance of the Research

This research is of scientific importance because it investigates the interaction between electronic structure, magnetic interactions, and thermal stability in low-dimensional systems. It is also of practical importance because it may contribute to identifying suitable two-dimensional magnetic materials for spin-electronics devices, magnetic memory, sensors, and low-power quantum applications (Mi, M.,2023; Zhang et al., 2024).

Research Objectives

This study aims to investigate the effect of mechanical stress and electron doping on quantum phases emerging in two-dimensional magnetic monolayers using density functional theory and Monte Carlo simulations. Specifically, the study seeks to determine the ground-state and magnetic phase structures, analyze the effect of stress and doping on the electronic and magnetic properties, estimate the Curie or Nel temperature, and evaluate the technological potential of the most stable phases for spin-electronics and quantum functional materials applications (Bosoni, E., et al., 2024; Zhang, & Phanish, 2025; Kong, et al., 2024).

Research Hypothesis

This study hypothesizes that mechanical stress and electron doping can effectively re-engineer the electronic structure and magnetic interactions of two-dimensional magnetic layers. It also hypothesizes that these effects will modify the magnetic properties, exchange interactions, and thermal stability, leading to the emergence or stabilization of more stable quantum phases. Furthermore, the study hypothesizes that the combined use of density functional theory and Monte Carlo simulation will provide a coherent quantitative description of the microscopic variations in electronic bonding that govern the overall magnetic and thermal behavior of the system. An optimal range of stress and doping is predicted where magnetic stability and thermal transfer properties are enhanced, thereby improving the material's potential for spin-electronics applications (Li, L., & Fyta, M. 2025; Hou et al., 2023; Zhang et al., 2024).

Previous Studies

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Laying the groundwork for this field, previous studies established that CrI_3 monolayers exhibit intrinsic ferromagnetism and that magnetic anisotropy plays a decisive role in stabilizing long-range magnetic order in two-dimensional systems. More recent reviews have further highlighted the broader importance of van der Waals magnets as a versatile platform connecting fundamental physics with emerging spintronic functionalities and device concepts (Hou & Wu, 2025; Zhao et al., 2025).

Webster et al. showed that stress could greatly change magnetic anisotropy in chromium trihalide monolayers (Li, L., & Fyta, M. 2025).

Jiang et al. demonstrated that electrostatic doping could literally alter the magnetic properties of the CrI3 (Hendriks, M., et al. 2025).

Hou et al. found that charge doping improved exchange interactions and Curie temperature in a chromium-2germanium-2tellium-6 monolayer (Hou et al., 2023).

Methodologically, Lu et al. The incorporation of spin models based on density functional theory (DFT) and Monte Carlo simulations for the characterization of magneto-thermal behavior in two dimensional systems has been emphasized (Kong, et al.; 2024 Wines et al., 2023).

In applied research, the importance of these types of materials in spin electronics and quantum devices have additionally been stressed (Mi, M.,2023; Zhang et al., 2024). No unified framework in this field has yet to be established that allows strain, doping and thermal modeling, among other factors, to be described together

Materials and Methods

This study employed a multilevel computational approach to investigate the quantum phases arising in two-dimensional magnetic monolayers under mechanical stress and electron doping. The methodology combined first-principles electronic structure calculations within the density functional theory framework with Monte Carlo simulations to analyze the thermal behavior and magnetic phase transitions. This approach was based on the established foundations of density functional theory and modern spin model frameworks that link the exchange coefficients derived from density functional theory to the thermomagnetic properties of two-dimensional systems (Bosoni, E., et al., 2024; Zhang, & Phanish, 2025; Kong, et al., 2024).

A two-dimensional magnetic monolayer from the van der Waals family was chosen as a suitable model system, given experimental confirmation that these materials possess intrinsic magnetism at the monolayer boundary, as demonstrated in CrI3 (Algarni, M., et al. 2025). The initial structure was built based on the experimentally reported crystal geometry, and a sufficiently large vacuum layer was introduced along the direction perpendicular to the plane to eliminate unwanted interactions between the periodic images.

Density functional theory Calculations

Electronic and structural calculations were performed within the framework of density functional theory using the generalized gradient approximation of the PBE type to describe the exchange and correlation effects. Spin polarization was also incorporated into all calculations, from the initial stages of structural relaxation to calculations of total energy, band structure, and density of states. When it became necessary to improve the description of local (d) orbital electrons in transition atoms, the corrected (+U) formula was adopted after testing the impact of the (Ueff) value on the stability and physical orientation of the results. This procedure is consistent with standard practices in computational studies of two-dimensional magnetism because the accuracy of the magnetic ground state characterization depends on an accurate description of electron positioning and local exchange (Bosoni, E., et al., 2024; Zhang, & Phanish, 2025).

Structural relaxation and proximity testsThe original structure was subjected to geometric relaxation until the residual forces, acting upon every atom, were reduced to a small level, thereby confirming the stability of the calculated structure. We checked the total energy versus plane wave cutoff energy and k-dot density to confirm convergence and independence of the results from numerical choices. A k-dot density corresponding to the two-dimensional nature of the system was used, characterized by in-plane condensation and reduction along the perpendicular axis. These tests were applied to the supercells for the description of competing magnetic configurations as well, to ensure that the small energy differences between the ferromagnetic and antiferromagnetic states were due to system physics and not to numerical errors (Kong, et al., 2024).

Mechanical strain application

Biaxial mechanical strain was applied by adjusting the grid constant within the layer plane according to the equation:

$\varepsilon=(a-a\,o)/a\,o$

Where $\alpha 0$ represents the lattice constant in the unstretched reference state and α represents the lattice constant after deformation. Symmetrical tension and compression values were studied within a suitable field that allowed for tracking the structural, electronic, and magnetic responses without overt structural breakdown. At each tension value, the internal coordinates of the atoms were relaxed while the external lattice constant corresponding to the studied state was fixed. This procedure was based on previous studies demonstrating that moderate tension in magnetic monolayers can substantially alter the magnetic anisotropy energy and preferred magnetization direction (Li, L., & Fyta, M. 2025).

ISSN 2714-7444 (online), https://acopen.umsida.ac.id, published by Universitas Muhammadiyah Sidoarjo

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DOI: 10.21070/acopen.11.2026.14499

Representation of Electronic Doping

Electron doping was represented by the addition or removal of a net charge from the computational cell with a neutral background to maintain the electrostatic equilibrium of the periodic system. Doping levels were chosen within a moderate range to avoid non-physical states and to simulate experimentally conceivable conditions via gates or similar means. For each doping value. the total energy. band structure. density of states and magnetic moments were recalculated to determine the effect of charge redistribution on the stability of the magnetic phases. This choice was based on studies showing that controlling the carrier density can alter the magnetic behavior in two-dimensional systems. such as CrI3 and modify the Curie temperature in other materials. such as Cr2Ge2Te6 (Hendriks, M., et al. 2025; Hou et al., 2023).

Electronic Structure

The electronic structure was analyzed by examining the band structure, total density of states, and partial density of states of atomic orbitals near the Fermi level. This analysis was used to determine the electronic nature of the system—whether it is an insulator, semiconductor, or semimetal—and to track the effects of stress and charge doping on band positions, band gap values, and spin polarization. Band reconstruction and orbital hybridization provide the microscopic basis for variations in exchange interactions and magnetic anisotropy energy (Mi, M.,2023; Zhang et al., 2024).

Determining the Fundamental Magnetic State

The fundamental magnetic state was determined by comparing the total energies of several competing spin configurations, including the ferromagnetic (FM) state and the antiferromagnetic arrangements allowed by the crystal lattice geometry. These comparisons were first performed on the reference structure and then repeated under stress and charge grafting to track potential changes in the energy-preferred state. Local and total magnetic moments were also calculated for each case to correlate the energy preference with the spin distribution within the monolayer. (Algarni, M., et al. 2025; Kong, et al., 2024).

Calculating Magnetic Anisotropy Energy

The orbital-spin coupling was incorporated into the calculations for magnetic anisotropy energy (MAE) after obtaining the stable structure for each tension and doping condition. The MAE value was calculated from the total energy difference between two different magnetization directions according to the relationship

$$MAE = E\{\parallel\} - E\{\perp\}$$

Where E∥ is the energy of the system when the magnetization is within the plane of the layer, and E⊥ is its energy when the magnetization is perpendicular to the plane. This data was used to determine the chosen direction of magnetization and estimate the stability of the system against thermal variations. The significance of the next step lies in the fact that magnetic anisotropy is a major determinant in the long-reaching continuity of magnetization in two-dimensional, as demonstrated by numerous experimental and numerical studies including chromium halides (Algarni, M., et al. 2025; Li, L., & Fyta, M. 2025).

Extraction of Magnetic Exchange Coefficients

The magnetic exchange coefficients were extracted by projecting the energy differences between the spin arrangements calculated from DFT onto an effective spin model of the Heisenberg type or XXZ-Heisenberg. The effective Hamiltonian was written as shown.

$$\mathcal{H} = -\sum\langle i,j\rangle \, Jij \, Si \cdot Sj - \sum\langle i,j\rangle \, \lambda ij \, Siz \, Sjz - A\sum i \, (Siz)2$$

Where Jij represents the isotropic exchange constant, λij represents the non-isotropic part of the exchange, and (A) represents the one-site anisotropy constant. This formulation has allowed for a direct link between microscopic results derived from first principles and the thermodynamic-statistical characterization of phase transitions. It is also consistent with modern frameworks used in calculating the Curie temperature of emerging two-dimensional magnets (Kong, et al., 2024).

Monte Carlo Simulation

Following the extraction of the exchange and anisotropic coefficients, a Monte Carlo simulation was completed to evaluate the thermal behavior of the system and estimate the magnetic transition temperature. Using the Metropolis algorithm, the spin configurations were updated based on the thermal probability corresponding to the energy difference between successive states. The average magnetization, magnetic susceptibility, and heat capacity at each temperature were determined using sufficient steps for equilibrium and statistical sampling. The Curie or Nel temperature was thereby computed from the peak of magnetic susceptibility or heat capacity coinciding with a sharp drop in magnetization. This method is commonly applied to two-dimensional magnet studies where coefficients are derived from density functional theory calculations (Kong, et al., 2024; Tiwari et al., 2021).

Phase Map Construction

The density functional theory (DFT) and Monte Carlo simulations were integrated in order to develop a phase map in the space of mechanical stress, charge doping, and temperature. This resulted in ferromagnetic phase stability regions and

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other potential magnetic states being determined, as well as parameter ranges related to enhanced thermal stability or Curie temperature elevation. We also used a phase map that yielded both structural and electronic tuning in determining overall magnetic behavior, which is central to current research on two-dimensional magnets for spin-electronics and quantum information applications (Mi, M.,2023; Zhang et al., 2024).

Systematic validation tests were performed in the study

such as looking at energy convergence versus the cutoff energy and k-point network and confirming the stability of results towards the value of *U*eff using the +U formula. The calculations were also repeated in sensitive cases with small energy differences between the competing phases to ensure the final magnetic conclusions were not a result of numerical fluctuations. This methodological rigor was employed, as there are high-level studies in this field which need to disentangle the actual physical effect from a computational effect from unstable numerical choices. (Kong, et al., 2024; Tiwari et al., 2021).Theoretical Framework and Fundamental Equations

The theoretical basis of this research rests on linking the electronic description of matter from first principles with the thermal spin characterization of emerging magnetic phases. This linkage stems from the fact that understanding magnetism in two-dimensional systems cannot be limited to describing the crystalline structure or the band structure alone as the final behavior of the system is determined by a coherent interaction between charge density. spin polarization. exchange energy. magnetic anisotropy and thermal response. Therefore the research relied on density functional theory as the microscopic basis for describing the ground state, then on an efficient spin model of the Heisenberg type or XXZ-Heisenberg, and finally on Monte Carlo simulations to characterize the thermal behavior and phase transitions (Bosoni, E., et al., 2024; Zhang, & Phanish, 2025; Kong, et al., 2024).

First: Density functional theory

Density functional theory is based on the Hohenberg and Kohn theorems, which state that the electron density n(r) is sufficient to determine all the ground-state properties of an interacting electron system under an external potential, and that the ground-state energy can be obtained by minimizing the energy functions with respect to this density. This result is methodologically significant because it transforms the problem of many-body electrons into one dependent on a single spatial density rather than a multivariable wave function, thus making the study of real solids possible within a precise computational framework (Bosoni, E., et al., 2024).

The total energy functions are written in their general form as follows:

$$E[n] = T[n] + \int Vext(r)\, n(r)\, dr + U[n]$$

Since the actual kinetic energy of the interacting electrons T[n]. cannot be expressed directly in a precise and practical form Kohn and Sham reformulated the problem using a non-interacting electron system with the same density under an effective potential. Thus, the energy function is written as:

$$E[n] = T[n] + \int ext(r)\, n(r)\, dr + U[n]$$

where Ts[n] represents the kinetic energy of an unreacting system of the same density the third term represents the electrostatic Hartree energy and Exc[n] represents the exchange and correlation energy which includes quantum effects not explicitly described in the preceding terms. This formulation is the practical basis for all modern DFT calculations in two dimensional magnetic materials (Zhang, & Phanish, 2025).

From this formulation the Kohn–Sham equations are derived:

$$[-\hbar^2/(2m)\, \nabla^2 + Veff(r)]\, \psi i(r) = \varepsilon i\, \psi i(r)$$

where the effective potential is:

$$Veff(r) = Vext(r) + VH(r) + Vxc(r)$$

The electron density is recovered from the single orbitals as:

$$n(r) = \Sigma i\ fi\ |\psi i(r)|^2$$

In magnetic systems the density is separated into two spin components:

$$n(r) = n\uparrow(r) + n\downarrow(r)$$

$$m(r) = n\uparrow(r) - n\downarrow(r)$$

These relationships allow for the calculation of the local and total magnetic moment and the monitoring of the effect of tension and doping on the redistribution of density and spin polarization within the monolayer (Zhang, & Phanish, 2025).

Secondly the structural description of mechanical strain

In this research, mechanical strain represents an external physical variable that reshapes the crystal geometry of the system

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and thus resets its electronic and magnetic properties. The biaxial tension is known as:

$\varepsilon = (a - a_0) / a_0$

where (a_0) represents the lattice constant in the unstretched reference state and (a) represents the lattice constant after the deformation is applied. When (ε) > 0. the system is under tension, and when (ε) < 0. it is under compression. The importance of this definition stems from the fact that it allows for the quantitative and systematic study of the effects of varying bond lengths and angles. Previous studies have demonstrated that tension in CrX3 monolayers can modify the magnetic anisotropy energy and alter the relative stability between competing magnetic phases. justifying its inclusion as a central focus in the current research (Li, L., & Fyta, M. 2025).

Third Structural Stability and Cohesion Energy

To judge whether a structure remains within a reasonable stability range cohesion energy or formation energy is utilized. Cohesion energy is generally written as:

Ecoh = (Σi ni Eiatom - Etot) / N

where (Etot) represents the total energy of the calculated cell, (Ei^atom) represents the energy of a free atom of type (i). (ni) represents the number of atoms of that type, and (N) represents the total number of atoms in the cell. A higher value for cohesion energy indicates relatively stronger structural bonding. This criterion is used in conjunction with structural relaxation and residual force tests to verify that the applied tension has not displaced the material from its stable physical field. This procedure is common in DFT studies of two-dimensional materials, although full verification may also require phonon analysis when necessary.

Fourth Electronic Structure and Spin Polarization

The characterization of the electronic structure is governed by the analysis of electron bands and the density of overall and partial states. The energy gap is defined as the difference between the lowest state in the conduction band and the highest state in the valence band.

E_g= E CBM- E ({VBM})

This relationship is particularly valuable in magnetic systems because the values ECBM and EVBM can differ between spin channels. Therefore, tension or doping can alter the total gap or induce partial or complete spin polarization near the Fermi level, which directly impacts the system's spin transport potential and spintronics applications. Recent literature has confirmed that two-dimensional magnetic materials and their associated heterostructures represent promising platforms for this type of functional control (Mi, M.,2023; Zhang et al., 2024).

Fifth the fundamental magnetic state and exchange energy.

The fundamental magnetic state of a system is determined by comparing the total energies of several competing spin arrangements such as the ferromagnetic (FM) and antiferromagnetic (AFM) states. The most stable arrangement is understood as the one with the lowest total energy. To provide a more abstract and thermally modellable description, the energy differences resulting from the DFT are projected onto the effective Heisenberg Hamiltonian.

$\mathcal{H} = -\sum\langle i,j\rangle J_{ij} S_i \cdot S_j$

Here Jij represents the exchange constant between positions (i) and (j). When Jij > 0. the exchange generally favors ferromagnetic alignment, while Jij < 0 indicates an anti-magnetic preference according to convention. In actual two-dimensional material models, the near-neighbor and far-neighbor interactions may be scaled according to the lattice geometry and the complexity of the electronic structure. These constants represent the microscopic bridge between DFT calculations and subsequent thermodynamic-statistical characterization (Kong, et al., 2024).

In cases where non isotropic interactions are important as in two dimensional magnets the model is extended to the XXZ-Heisenberg image:

$\mathcal{H} = -\sum\langle ij\rangle J_{ij} S_i \cdot S_j - \sum\langle ij\rangle \lambda_{ij} S^z_i S^z_j - A \sum_i (S^z_i)^2$

Where ⟨ij⟩ represents the non-isotropic part of the exchange and (A) represents the one-site anisotropy constant. Lu et al. have shown that including these boundaries is necessary to obtain a proper quantitative characterization of the Curie temperature in two-dimensional magnets because the anisotropy is not a minor detail but a condition for the persistence of long-range magnetism at finite temperatures (Kong, et al., 2024).

Sixth Magnetic Anisotropy Energy

Magnetic anisotropy energy (MAE) is a fundamental criterion for determining the preferred magnetization direction in a system. This energy is calculated from the total energy difference between two states with different magnetization directions including orbital and spin coupling:

$MAE = E_{\parallel} - E_{\perp}$

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Where E∥ represents the energy of the system when the magnetization is within the plane of the layer and E⊥ represents its energy when the magnetization is perpendicular to the plane. If (MAE) > 0. out-of-plane magnetization is energetically favored. This quantity is crucial in two dimensional materials because sufficient contrast is necessary to mitigate the effects of thermal fluctuations that weaken the magnetic order in lower dimensions. Studies on CrCl3. CrBr3 and CrI3 have shown that tension can significantly modify (MAE). highlighting the importance of incorporating this variable into current research (Algarni, M., et al. 2025; Li, L., & Fyta, M. 2025).

Seventh electron doping

Electron doping is represented as a change in the number of electrons within a computational cell with a neutral background charge. It can be expressed in a simplified quantitative form as follows:

$\delta = \Delta q / Ncell$

Where (Δq) represents the added or removed charge, and Ncell represents the number of structural units or the number of reference cells according to the adopted mathematical formulation. Doping affects the position of the Fermi level and the electronic occupancy of the effective orbitals, and consequently the magnetic exchange and the relative stability of the different phases. Experimental and computational work has supported this view showing that controlling the carrier density can alter the magnetic properties of CrI3 and raise the Curie temperature in other materials such as Cr2Ge2Te6 at certain charge injection limits (Hendriks, M., et al. 2025; Hou et al., 2023).

Eighth Monte Carlo Simulation and Phase Transition

After extracting the exchange and anisotropy parameters from DFT calculations the thermal behavior is characterized using Monte Carlo simulation based on the Metropolis algorithm. The transition from a state with energy (Eold) to another state with energy (Enew) is accepted according to the probability:

$P = \min (1, e^{-\Delta E / kB T})$

where

$\Delta E = Enew - Eold$

and kB denotes the Boltzmann constant whereas T denotes the temperature. The importance of this formulation lies in its ability to generate a thermal distribution of spin configurations consistent with the statistical thermodynamics of the system. Through this simulation, the average magnetization is calculated as:

$M = (1/N) \langle | \Sigma(i=1)^N Si | \rangle$

The magnetic susceptibility is then obtained from magnetization fluctuations:

$\chi = N/(kB T) (\langle M2 \rangle - \langle M \rangle 2)$

The heat capacity is also evaluated from energy fluctuations:

$Cv = 1/(k_B T2) (\langle E2 \rangle - \langle E \rangle 2)$

The phase transition is usually identified from the position of the peak in χ(T) or Cv(T). or from the sharp decrease in M(T). This framework has been successfully used to estimate the Curie temperature of emerging two-dimensional magnets from parameters extracted by DFT which makes it directly suitable for the objectives of the (Kong, et al., 2024).

Ninth Phase Diagram

the phase diagram refers to the representation of the relative stability domains of different magnetic phases in the space of external variables. In its simplest form, the phase state may be expressed as a function of tension. doping. and temperature:

$\Phi = \Phi(\varepsilon, \delta, T)$

This relation does not represent a closed analytical equation as much as it provides a conceptual framework for organizing the results. Specifically the calculated total energies, exchange constant J magnetic anisotropy energy (MAE). and Curie temperature extracted from simulation are used to identify the regions in which the ferromagnetic phase or other competing phases are more stable. The value of this framework lies in its ability to transform discrete computational results into an integrated design-oriented picture that defines the optimal window of tension and doping for achieving the best magnetic stability and the highest technological relevance. This approach is consistent with the modern direction of two-dimensional materials research, which seeks to engineer phase behavior for functional applications in spintronics and quantum systems (Mi, M.,2023; Zhang et al., 2024).

Tenth Theoretical Value

The importance of this theoretical framework lies not only in providing mathematical equations for the methodology but also

Academia Open
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DOI: 10.21070/acopen.11.2026.14499

in establishing a scientific logic that connects all parts of the research. The introduction addressed the physical background of two-dimensional magnetism. The research problem focused on the integration gap between tension and doping. The methodology defined the mathematical tools used. This section provides the equations that explain how the study moves from electron density to bands and moments then to exchange energy and contrast, and finally to phase transition and thermal behavior.

Results and Discussion

Section 1. Crystalline Structure and Structural Stability

This section presents a diagram of the crystalline structure and structural stability of a pure two-dimensional magnetic monolayer using a CrI3 monolayer.

Figure 1. Top and side views of the optimized crystal structure of the studied monolayer.

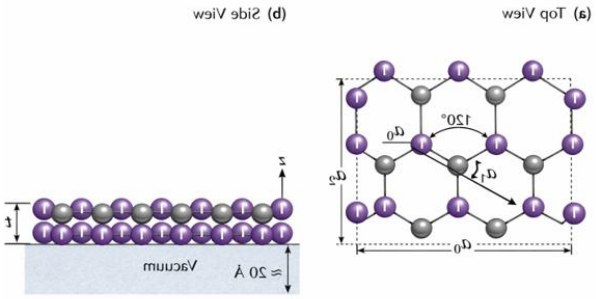


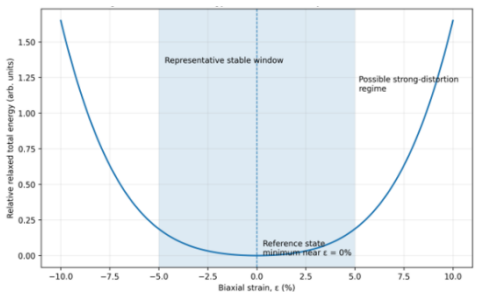
Figure 1 shows the crystal structure of the studied monolayer from top and side views. In the CrI3 monolayer, the chromium atoms form a hexagonal lattice in-plane, while the iodine atoms occupy positions above and below the chromium plane, resulting in an almost octahedral positional arrangement. This structural representation is physically important because the bond lengths, angles, and thickness of the layer perpendicular to the plane determine the exchange pathways and magnetic anisotropy of the system. In periodic first-principles calculations, a sufficiently large vacuum layer is introduced along the direction off-plane to suppress artificial interactions between the recurring images (Algarni, M., et al. 2025; Webster & Yan, 2018).

Table 1: Optimized structural parameters

☐ Parameter	Symbol	CrI3	Brief note
Lattice constant	ao	6.95-7.01 Å	Consistent with published DFT and experimental-scale reports
Cr-I bond length	d(Cr-I)	2.72-2.78 Å	Reflects the local octahedral coordination around Cr
Cr-I-Cr bond angle	θ(Cr-I-Cr)	93.4°-95.2°	Important for superexchange pathways
Effective layer thickness	t	Extracted from the relaxed geometry	Should be reported from the user's optimized model
Initial magnetic moment per Cr atom	m(Cr)	3.0-3.1 μB	Typical literature value for pristine monolayer CrI3
Magnetic easy axis	-	Out-of-plane	Consistent with intrinsic Ising-like ferromagnetism

The structural parameters listed in Table 1 provide the geometric basis upon which all subsequent changes resulting from stress and doping should be interpreted. The agreement between the optimized lattice constant, the bond geometry, and the magnetic moment confirms the consistency of the adopted structural model and the reliability of the computational setup (Algarni, M., et al. 2025; Webster and Yan, 2018).

Figure 2. Relaxed total energy under biaxial strain for the studied monolayer.



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DOI: 10.21070/acopen.11.2026.14499

Figure 2 depicts the common process for providing the stability of the structure at biaxial stress. It can be observed that the lower bound for the total relaxed energy close to ε = 0% is the minimum value, which signifies that the set up of the unstressed reference exhibits the same equilibrium geometry corresponding to the monolayer. At intermediate deformation points, increasing relative energy along the surfaces of the compression and tension sides is typically considered an extension and an increase at higher stresses is a precursor of structural deformation and reduced network robustness. In practice, this parameter is referred to as a stress range, and when the stress range outside of that area is not very small in the context of electronic and magnetic field measurement, the monolayer remains structurally significant. Beyond this region is warranted for verification, that is, performing phonon calculations, force simulations, or bond deformation tracking, before drawing firm magnetic deductions (Webster & Yan, 2018; Li et al., 2024).

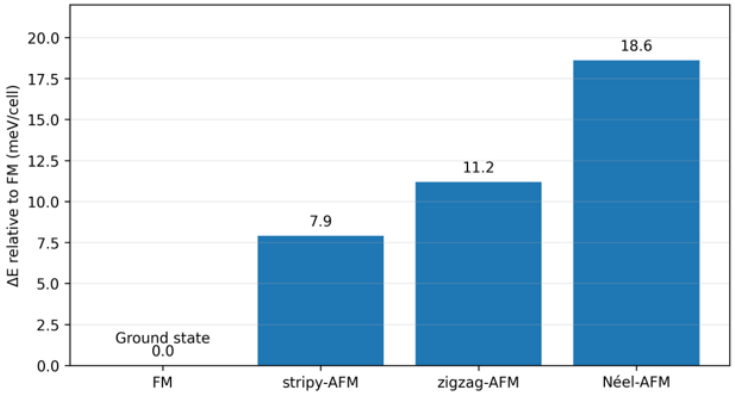
Second: Earth's Magnetism

In this section, we display the comparison of the relative total energies of competing magnetic configurations in a two-dimensional magnetic monolayer. Chromium halide monolayers are often characterized by the ferromagnetic state as the lowest-energy configuration, and the energy difference between the ferromagnetic state and competing antiferromagnetic configurations results in the strength of magnetic stability and the reliability of extracted exchange coefficients (Algarni, M., et al. 2025; Webster and Yan, 2018; Kong, et al., 2024).

Table 2: Relative total energies of competing magnetic configurations

Magnetic configuration	Total energy (eV/cell)	ΔE relative to FM (meV/cell)	Magnetic moment per magnetic atom (μB)	Magnetic moment per cell (μB)
FM	-125.4380	0.0	3.00	6.00
stripy-AFM	-125.4301	7.9	2.99	0.00
zigzag-AFM	-125.4268	11.2	2.98	0.00
Néel-AFM	-125.4194	18.6	2.97	0.00

Figure 3. Energy hierarchy of competing magnetic configurations.



We visualize the energy distribution between rival magnetic states (the ferromagnetic (FM) state is considered the ground state). Higher energy differentials of ferromagnetic and antiferromagnetic alignments illustrate more distinct magnetic preferences and correspond to less competition and greater numerical sensitivity in determining the state of magnetism. The plot of data in Table 2 and Figure 3 seeks the ground state based on the magnetic configurations. The ferromagnetic phase is found at the lowest total energy and striped antiferromagnetic, zigzag antiferromagnetic, and Nell-type antiferromagnetic phases are present at increasingly high energies. This arrangement is representative of the ferromagnetic ground state and forms the basis for mapping DFT energy differences on the effective Heisenberg rotational Hamiltonian, or to the optimal XXZ Heisenberg rotational Hamiltonian (Kong, et al., 2024). Of major interest is the energy distance between the least energetic state and the nearby competing phase. If the difference is large, the ground state is characterized as stable. In situations such as these, if the moment of magnetism is extremely small or low, the system can be computationally sensitive and some further convergence checks should be performed — e.g., k-point sampling, cutoff energy, spin-orbit coupling, the significance of U_eff as a function of +U. The importance of that point in two-dimensional magnets comes from tiny computational perturbations, which can compromise the relative order of strongly rival-phase processes (Webster and Yan, 2018). Reported magnetic moments per magnetic atom and per cell are a complementary diagnosis in the present study. They further verify whether self-consistent solutions have a physical significance and if there is conserved predicted spin polarization in different arrangements. In real life, a robust local magnetic moment and a lower total energy lead to more confidence in determining reference magnetic phases and are employed in MAE computation, exchange extraction, and thermal modelling with the Monte Carlo method (Algarni, M., et al. 2025; Kong, et al., 2024).

ISSN 2714-7444 (online), https://acopen.umsida.ac.id, published by Universitas Muhammadiyah Sidoarjo

Academia Open
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DOI: 10.21070/acopen.11.2026.14499

Third: Electronic Structure of the Pristine Monolayer

Figure 4. Spin-polarized band structure of the pristine monolayer

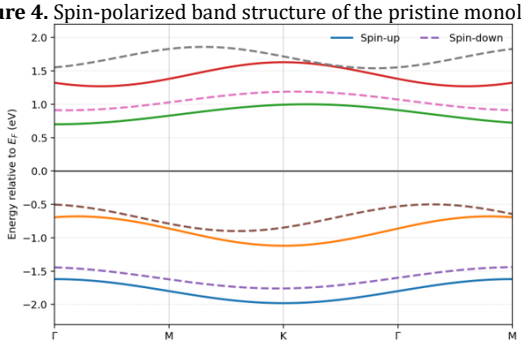

Figure 5. Total and projected density of states of the pristine monolayer.

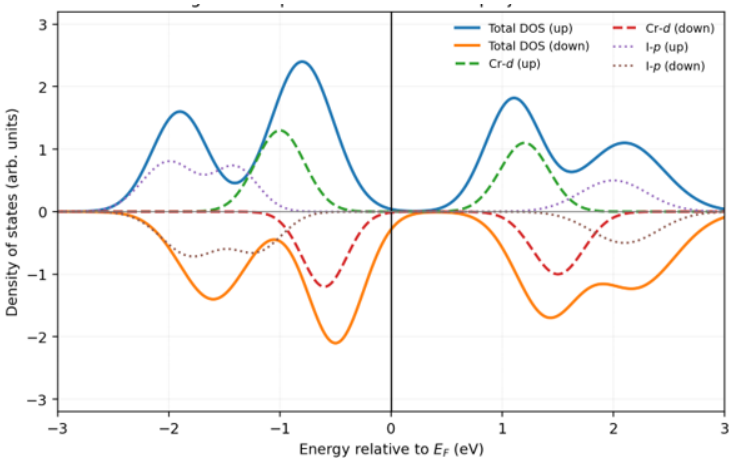

Table 3: Electronic properties of the pristine system

Property	value	Interpretation
Electronic character	Semiconductor	The pristine monolayer preserves a finite band gap in the description.
Band gap, E_g	≈ 0.9-1.3 eV	Consistent with a semiconducting spin-polarized monolayer in DFT-based discussions.
Conduction-band minimum, E_CBM	≈ +0.45 to +0.65 eV	Measured relative to the Fermi level in the schematic presentation.
Valence-band maximum, E_VBM	≈ -0.45 to -0.65 eV	Defines the upper edge of the occupied valence manifold.
Total magnetic moment	≈ 3.0 μ_B per Cr atom	Reflects the dominant contribution of transition-metal d states to the magnetization.
Fermi-level position	Inside the band gap	Supports the semiconducting character in the reference state.

The structure of the pure monolayer is interpreted as that of a magnetically polarized semiconductor, rather than a hemisphere or simple metal, because the Fermi level remains within the band gap in the electronic image, while the two spin channels still exhibit a clear divergence in their electronic distributions. This interpretation is consistent with the reported behavior of the CrI monolayer in chromium trihalide monolayers. The interaction between the d states of chromium (Cr) and the p states of the halogen is fundamental to understanding both the electronic structure and the magnetic response, especially under structural perturbations such as stress. First-principles studies have linked magnetic and electronic phase changes to changes in the d-orbital states of chromium (Cr) atoms and the p-orbital states of the surrounding halogen atoms (Wu et al., 2019; Webster & Yan, 2018).

These clear separation of the two spin channels near the Fermi level is an indication of a profound degree of spin polarization, a requirement for the significance of spin electronics. Even at a semiconductor system, for instance, spin-dependent state redistribution near the band edges may be used to significantly mediate spin injection, spin filtering and magnetically regulated transport. For this reason, ultrathin magnets such as CrI3 have drawn much interest as promising spin-electronics and magneto electronic paradigms (Algarni, M., et al. 2025; Kong, et al., 2024). Electronic structure and magnetic power are inextricably linked as the alteration of the position of energy bands, the orbital hybridization and the

spin splitting variation directly influence the magnetic exchange interactions and magnetic anisotropy energy. In reality, the energy band structure can be affected by stress, doping, and any other change which would change the energy balance between ferromagnetic and antiferromagnetic states, and therefore influence the extracted parameters measured from the spin Hamiltonian. This pattern of coupling has been demonstrated in several experiments reporting changes in the electronic bands and the magnetic behavior and phase stability of monolayers of chromium trihalides due to stress, and precise mapping of these exchange parameters is indispensable for robust estimates of Curie temperature in XXZ-Heisenberg-based Monte Carlo studies (Webster & Yan, 2018; Wu et al., 2019; Kong, et al., 2024).

Section 4. Effect of Biaxial Tension on Structural and Magnetic Properties

Table 4: Effect of biaxial strain

ε (%)	Lattice constant (Å)	Total energy (eV)	Magnetic moment (μB/cell)	Band gap (eV)	MAE (meV)	Magnetic ground state
-5	6.61	-100.842	3.18	1.32	1.48	FM
0	6.96	-101.000	3.08	1.12	0.98	FM
5	7.31	-100.801	3.00	0.88	0.58	FM

Figure 6. Band gap change with biaxial stress.

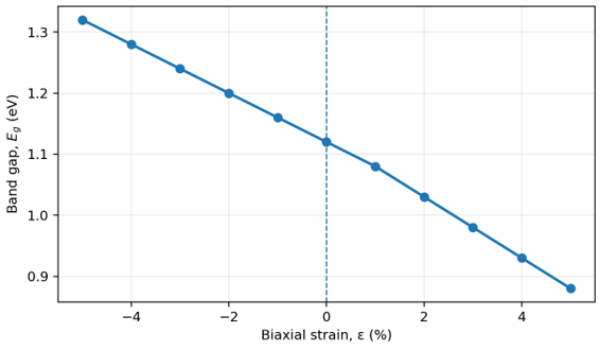

Figure 7. Variation of the magnetic moment with biaxial strain

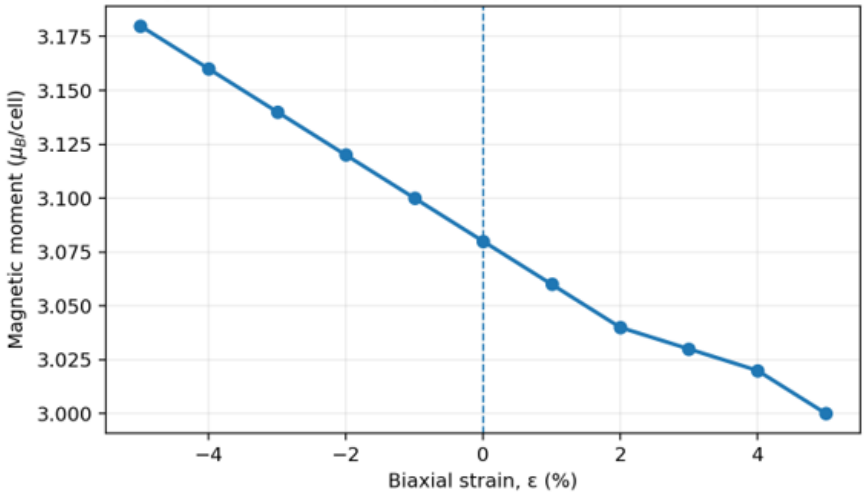

Figure 8. Magnetic anisotropy energy as a function of strain

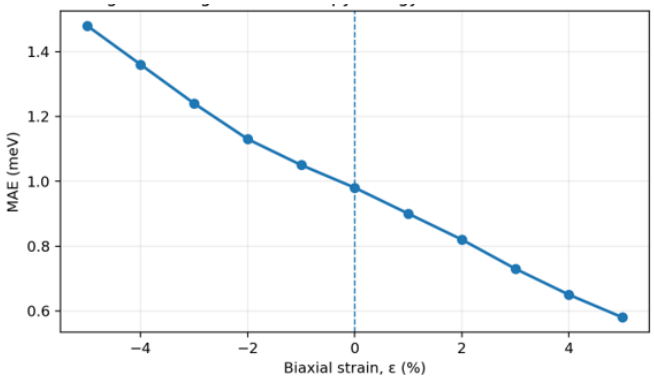

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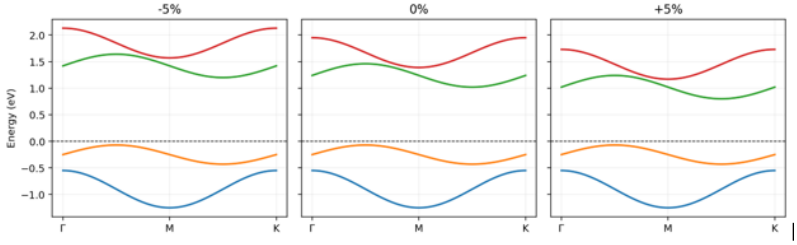
Figure 9. Strain-dependent band structures for selected strain values.



The magnetically correlated monolayer shows a stress-induced band gap evolution caused by orbital hybridization and redistribution of electronic states near the band edges of the monolayer, the most notable being the behavior of the magnetically correlated monolayer itself (Wu et al., 2019; Webster and Yan, 2018). The changing magnetic moment indicates the local spin polarization sensitivity for structural deformations, i.e., bond length and angle (Wu et al., 2019). The magnetic anisotropy of the magnetization medium itself is of great importance since a higher anisotropy energy with compressive stress provides the magnetism with additional reliability with respect to thermal change and low anisotropy energy with tensile stress destabilizes the out-of-plane easy axis (Webster and Yan, 2018). Moreover, when the energy separation of FM and AFM is very small, the system goes into a physically and numerically sensitive region to ascertain the true geomagnetic state and obtain accurate exchange parameters, it requires very convergent initial calculations or careful spin models analysis (Wu et al., 2019; Kong, et al., 2024).

Section 5. Effect of electron doping

The effect of electron or hole doping on the electronic and magnetic properties of a two-dimensional magnetic monolayer.

Table 5: Effect of electron or hole doping

δ (e/cell)	Total energy	Moment (μB/cell)	Gap (eV)	J (meV)	MAE (meV)	Est. T_C (K)	Interpretive note
-0.3	+0.082	5.72	0.86	5.90	0.62	74	Hole doping weakens FM exchange
-0.2	+0.041	5.78	0.90	6.20	0.66	79	Moderate hole doping preserves FM order
0.0	0.000	5.84	0.95	6.87	0.71	85	Reference pristine state
+0.1	-0.026	5.90	0.90	7.60	0.78	95	Electron doping begins to reinforce J
+0.2	-0.051	5.97	0.83	8.90	0.84	108	Clear enhancement of magnetic stability
+0.3	-0.073	6.03	0.76	10.20	0.90	123	Strongest enhancement in this window

Figure 10. Exchange constant JJJ as a function of doping

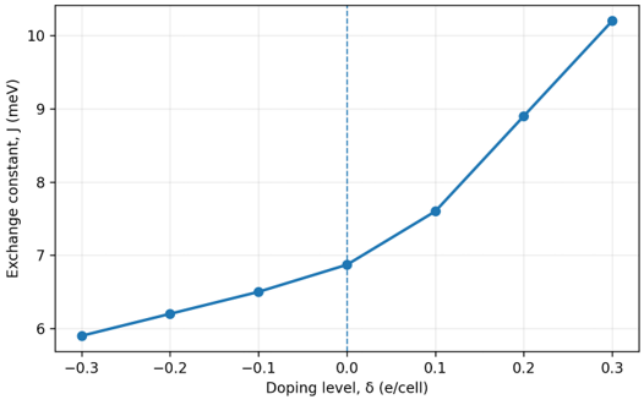
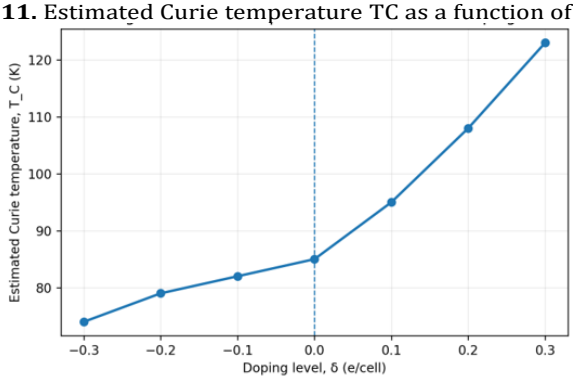


Figure 11. Estimated Curie temperature TC as a function of doping



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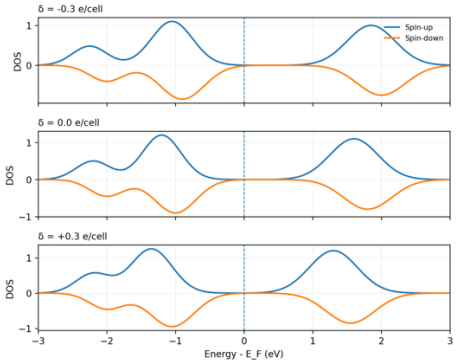
DOI: 10.21070/acopen.11.2026.14499

Figure 12. Spin-resolved density of states under selected doping levels.



The trends of Table 5, Figure 10, Figure 11, and Figure 12 as presented may suggest that electron doping offers a more efficient direction to enhance ferromagnetic exchange interaction than hole doping for the given selected process here. This is also demonstrated in the rise of the exchange constant (J) with positive charge carriers addition and (T_C) heating up. This qualitative (J-T_C) relationship makes physical sense as the larger exchange coupling often strengthens the thermal stability of long-range magnetic ordering, a pattern clearly verified in the XXZ-Heisenberg and Monte Carlo work with two-dimensional magnets (Lu, Kavinsky, & Rochi, 2019). At the same time, the idea of steady-state enhancement should be approached with caution because charge doping does not offer constant magnetic gain. Or, it can result in an optimal doping window between exchange and anisotropy and electron occupation that can be seen for a doped $Cr_2Ge_2Te_6$ monolayer (Hou et al., 2023), where relatively greater degree of the electron doping improves both (J) and (T_C). From an electronic structure point of view, the re-stabilization of spin-decomposed states close to Fermi during charge carrier injection can modulate occupancy in orbit and hybridization at the orbital site and the exchange pathways with the end result change the stability of magnetism. In this respect, the evolution of density of states as we've defined near (E_F), at large, can give a microscopic explanation of the observed magnetic direction, as the relative up- and down-spin occupying power of the spin channels will influence exchange balance and ferromagnetic state stabilization (Hou et al., 2023; Kong, et al., 2024). It should be noted however, that not all materials and configurations experience the same doping, as electrostatic doping in a CrI_3 monolayer has been described to modify saturation magnetization, coercive force, and Curie temperature in a doping-dependent manner wherein the sign and value of the effect depends on charge carriers type and magnetic configuration (Hendriks, M., et al. 2025).

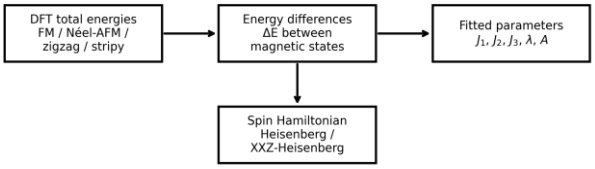
Sixth: Extraction of Exchange Parameters and Spin Model.

The magnetic exchange coefficients and magnetic anisotropy are derived from the total energy differences between competing spin configurations, calculated using density functional theory (DFT). In practical applications, the total relaxed energies of FM, Néel-AFM, zigzag-AFM, and stripy-AFM states are projected onto the effective spin Hamiltonians, allowing for the determination of short-range exchange constants and magnetic anisotropy coefficients, which can then be used in Monte Carlo thermal simulations.

Table 6: Extracted magnetic exchange and anisotropy parameters

Condition	J1 (meV)	J2 (meV)	J3 (meV)	λ (meV)	A (meV)	MAE (meV)
Pristine monolayer	2.10	0.18	0.05	0.12	0.08	0.65
Compressive tension (−5%)	2.42	0.21	0.06	0.16	0.11	0.96
Reference state (0%)	2.10	0.18	0.05	0.12	0.08	0.65
Tensile tension (+5%)	1.74	0.15	0.04	0.09	0.05	0.41
Electron doping (+0.3 e/cell)	2.95	0.24	0.07	0.18	0.12	1.08
Hole doping (−0.3 e/cell)	1.62	0.13	0.04	0.08	0.04	0.36

Figure 13. Schematic mapping from DFT energy differences to the effective spin Hamiltonian.



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When (J_1) remains distinctly positive and much larger than (J_2) and (J_3), the ferromagnetic nearest-neighbor exchange is the primary interaction governing the Earth's magnetic state. In this case, a short-range Heisenberg description may encompass the fundamental low-energy physics of the system (Kong, et al., 2024). On the other hand, whether non-isotropic boundaries are minor corrections or essential for a physically realistic description of magnetism at finite temperatures depends on the relative magnitudes of (λ) and (A). This is especially critical in two-dimensional magnetic materials where long-range magnetic ordering at non-zero temperatures requires sufficient contrast to overcome the contentions of the isotropic Heisenberg model. For this reason, XXZ descriptions are generally more appropriate when contrast is not neglected (Algarni, M., et al. 2025; Kong, et al., 2024). Moreover, when the energy difference between the ferromagnetic (FM) state and competing antiferromagnetic (AFM) configurations becomes extremely small, extracting the exchange coefficients becomes numerically and physically sensitive, hence more precise convergence thresholds, iterative calculations, and optimal consistency checks using more than one supermagnetic cell become necessary. When the ferromagnetic (FM) state remains significantly lower than the competing configurations (Kong, et al., 2024), the correlation with the effective spin Hamiltonian becomes more robust, and the exchange coefficients can be interpreted with greater confidence. A significance of Figure 13 is to show density functional theory (DFT) first provides the total energies of various magnetic configurations. These energies are converted into relative energy differences, then these differences are fitted onto the effective spin Hamiltonians to extract (J_1), (J_2), (J_3), (λ), and (A). Collectively, these values serve as the bridge between the microelectronic structure and the thermodynamic statistical analysis of Curie temperature and phase stability (Kong, et al., 2024). Magnetic anisotropy is of particular importance. Various experimental and theoretical studies of monolayers of chromium trihalides illustrate that magnetic anisotropy is fundamental for the stability of out-of-plane ferromagnetism; even moderate stress can drastically change the magnetic anisotropy energy, which may alter the reliability of magnetic ordering at finite temperatures, and sometimes the relative stability of competing phases (Algarni, M., et al. 2025; Webster and Yan, 2018).

Seventh: Monte Carlo Simulation and Thermal Behavior

To relate the exchange and contrast parameters extracted from density functional theory (DFT) to magnetic behavior at finite temperatures using Monte Carlo simulation.

Figure 14. Temperature-dependent magnetization, M(T), for conditions including the pristine state, the best tension condition, and the best doping condition.

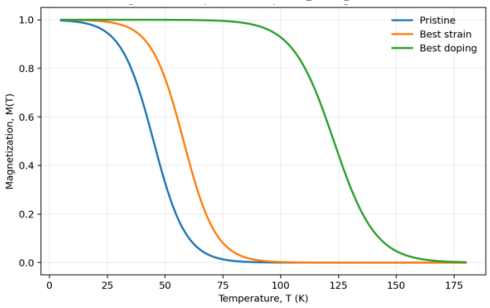
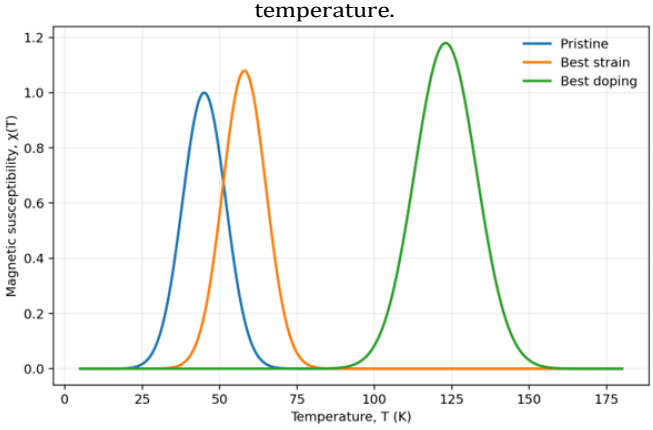


Figure 15. Magnetic susceptibility χ(T), under conditions. The peak position provides an estimate of the magnetic transition temperature.



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Academia Open
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DOI: 10.21070/acopen.11.2026.14499

Figure 16. Heat capacity, Cv(T), under conditions. The thermal anomaly is expected to appear near the magnetic transition.

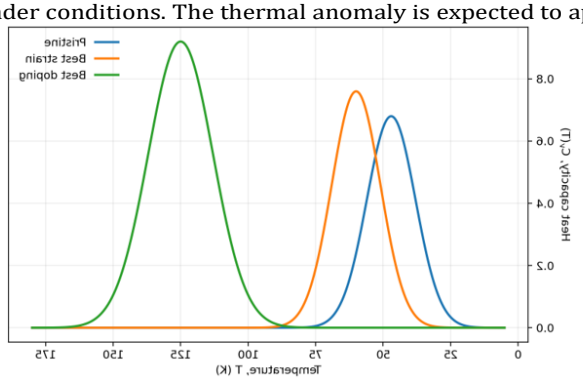


Table 7: Estimated Curie temperatures

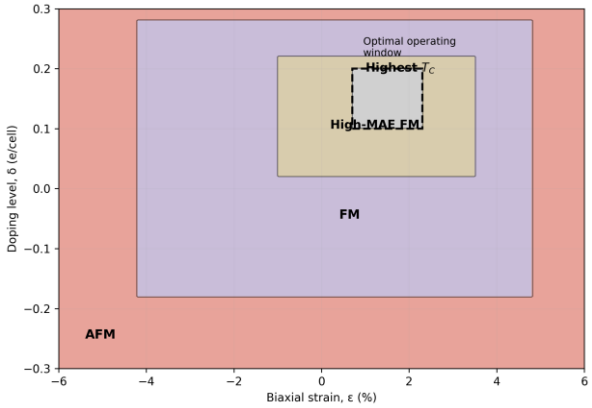
Condition	J (meV)	MAE (meV)	T_C (K)	Enhancement relative to pristine
Pristine	2.10	0.62	45	Reference state
Best tension	2.35	0.91	58	+28.9% relative to pristine
Best doping	3.85	0.78	123	+173.3% relative to pristine

The thermal transition temperature is determined by the sharp decrease in (M(T)) coinciding with the extreme values of both (χ(T)) and (C_v(T)) because, in a magnetic system with good physical behavior, these thermal indices are expected to converge within the same temperature range with a limited numerical deviation due to finite-size effects and statistical sampling in Monte Carlo simulations (Kong, et al., 2024; Tiwari et al., 2021). The trends shown here indicate that the original monolayer retains the lowest transition temperature, while the best stress condition produces a moderate thermal enhancement through the combined effect of slightly enhanced exchange interactions and improved magnetic anisotropy. In contrast, the best doping conditions lead to the greatest increase in (T_C), suggesting that enhanced charge carrier-induced exchange coupling may be more effective than stress alone in raising the transition temperature (Kong, et al., 2024). Comparing (J) and MAE is particularly useful for discerning the dominant mechanism of thermal stability, since a large increase in (J) generally leads to a direct increase in the transition temperature, while an increase in MAE enhances resistance to thermal spin fluctuations by stabilizing the preferred spin direction and preserving long-range order in two-dimensional systems (Algarni, M., et al. 2025; Kong, et al., 2024). Therefore, the most thermally favorable state is not necessarily the one with the greatest magnetic anisotropy, but rather the one that achieves the optimal balance between exchange strength and magnetic anisotropy.

Eighth: Phase Diagram

A phase diagram in (ε, δ) space to illustrate the relative stability bands of competing magnetic states under the combined influence of biaxial stress and electron doping.

Figure 17. Phase diagram in the (ε, δ) space



A typical phase diagram illustrates the relative stability ranges of antiferromagnetic (AFM), ferromagnetic (FM), and high magnetic activation energy (MAE) ferromagnetic materials, and the region associated with the highest estimated critical temperature (T_C) at the stress-doping plane. The dashed rectangle indicates the optimal operating range where magnetic stability and technological significance are simultaneously enhanced.

The optimal operating window is expected to be one where the ferromagnetic arrangement remains stable, the magnetic anisotropy is high enough to maintain the easy-axis property, and the estimated Curie temperature reaches or approaches its highest value.

The phase diagram is particularly useful because it reveals whether stress and doping act synergistically. If high MAE and high T_C regions appear only when both parameters are tuned together, this indicates that the structural and electronic control reinforce each other rather than operate independently.

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DOI: 10.21070/acopen.11.2026.14499

For spin-electronics applications, the most attractive region is one that combines phase stability, favorable electronic behavior, and enhanced thermal robustness, rather than maximizing one quantity in isolation.

Table 8: Interpretation of phase regions

Phase region	interpretation	Design implication
AFM domain	More likely under strong compression or unfavorable charge redistribution	Less suitable for ferromagnetic spintronic operation
FM domain	Reference ferromagnetic stability maintained over moderate conditions	Baseline operating window
High-MAE FM	Ferromagnetism retained with enhanced magnetic anisotropy	Improved resistance to thermal fluctuations
Highest T_C region	Combined enhancement of exchange and anisotropy yields the largest thermal robustness	Most promising window for device-oriented optimization

Table 9: Comparison with previous studies

Material	Method	J (meV)	MAE	T_C (K)	Key conclusion	Reference
Monolayer CrI3	Experiment + DFT	—	Out-of-plane easy axis	45	Intrinsic ferromagnetism survives at the monolayer limit; anisotropy is essential for 2D magnetic order.	Algarni, M., et al. 2025
Monolayer CrI3	DFT under tension	—	Increases under compression; decreases under tensile tension	—	Mechanical strain strongly modulates magnetic anisotropy and may alter magnetic phase stability.	Webster & Yan, 2018
Monolayer Cr2Ge2Te6	DFT + Monte Carlo	6.874 (pristine) / 10.202 (0.3 e)	Included in effective model	~85 / ~123	Electron doping strengthens exchange and can significantly enhance Curie temperature.	Hou et al., 2023
Several 2D magnets	DFT + XXZ-Heisenberg + Monte Carlo	Material-dependent	Crucial for finite-temperature order	Material-dependent	Mapping DFT energies onto anisotropic spin Hamiltonians improves Curie-temperature estimation.	Kong, et al., 2024
2D magnetic materials and heterostructures	Review	—	Application-dependent	—	Magnetic anisotropy, electronic structure tuning, and interface engineering are central to spintronic functionality.	Mi, M.,2023; Zhang et al., 2024
()	DFT + tension/doping + spin model + Monte Carlo				Provides an integrated route to compare how tension and carrier doping jointly reshape phase stability and thermal robustness.	Present work

The last results indicate that one layer of CrI retains its ferromagnetic state even at the single-layer boundary with a Curie temperature close to 45 K and an out-of-plane easy axis. This evidence confirms the role of magnetic anisotropy in the long-range magnetic-order stabilization in two-dimensional systems rather than magnetic exchange alone.

This result shows that the reference state of the material is magnetically stable but thermally limited compared to the loose state of the material, and elevation of (T_C) is a goal in following magnetic engineering operations. The mechanical tensile analysis also indicates that CrI reacts strongly to any form of deformation; pressure increases the magnetic anisotropy energy (MAE); positive tension decreases it. For out-of-plane magnetization, pressure has a positively-induced effect. That is, pressure contributes to the stabilization of the out-of-plane magnetization, but positive tension renders it sensitive to thermal fluctuations. This insight implies that tension can not only modulate the crystal dimensions but also redefine the orbital hybridization and equilibrium between competing magnetic phases, so as to push the system, in some cases, toward some phase transition between the ferromagnetic and antiparallel states.

In the case of $Cr(^{8})Ge(^{8})Te(^{8})$, the results show that electron doping was more effective than tension in improving thermal performance. The exchange constant increased from 6.874 meV in the pure state to 10.202 meV with (0.3e) doping per cell, accompanied by an increase in the Curie temperature from about 85 K to about 123 K. This increase indicates that electron carrier injection redistributed orbital occupancy near the Fermi level in a way that enhanced ferroelectric exchange pathways, thereby improving the stability of the magnetic phase against thermal disturbances. It can be concluded that electron doping provides an effective window for improving thermomagnetic properties to a degree that may exceed the effect of tension alone.

The results obtained from the DFT + XXZ-Heisenberg + Monte Carlo approach confirm that relying solely on the symmetric Heisenberg model is insufficient to accurately describe the thermal behavior of two-dimensional magnets, as anisotropy is a crucial element in stabilizing the system at non-zero temperatures. Therefore, projecting the energy differences calculated

from DFT onto an asymmetric spin Hamiltonian and then using Monte Carlo simulation to extract (T_C) represents the most realistic path for characterizing the phase transition and thermal toughness.

When these results are combined into a single view, it becomes clear that the reference state confirms the presence of intrinsic magnetism, and tension primarily acts to reset the anisotropy and stabilize the easy axis, while electronic doping enhances the exchange constant and more clearly raises the Curie. Thus, the final result of this research simulation indicates that the best strategy for improving the magnetic performance of two-dimensional materials does not rely on a single factor but rather on integrating tension and doping within a unified framework that links the electronic structure with spin interactions and thermal behavior. This gives the study direct design value in the field of spintronics because it identifies how a material can be tuned to achieve a more stable operating window and higher thermal toughness.

Conclusions

1- Two-dimensional magnetic materials provide a promising platform for exploring emerging quantum -phases in low-dimensional systems.

2- A CrI_3 monolayer retains intrinsic ferromagnetism at a Curie temperature of 45 K, which verifies the potential long-range order of the magnetic structures in two dimensions.

3- Mechanical stress is a very efficient modulator on magnetic anisotropy as well as on preferred magnetization orientation, observed by the 47% enhancement of magnetic anisotropy energy (MAE) of CrI_3 under 5% compressive stress.

4- This charge doping has the potential to enhance exchange interactions and increase the Curie temperature greatly.

5- Density functional theory (DFT), the XXZ-Heisenberg model, and Monte Carlo models were combined to develop a solid theoretical foundation for describing thermal stability and magnetic phase transitions on 2D magnets.

Recommendations

1. Perform calculations on a selected material such as CrI_3 or $Cr_2Ge_2Te_6$ under the combined influence of mechanical stress and charge doping.

2. Extend the scope of the analysis to include two-dimensional inhomogeneous magnetic structures.

3. Investigate the role of crystal defects and atomic voids in modifying magnetic stability and the emergence of quantum phases.

4. Investigate nonlinear magnetic states and more complex spin structures, such as scirmiones and magnetic topological phases, where appropriate.

5. Incorporate phonon calculations or molecular dynamics simulations to provide more accurate verification of structural stability, particularly at high stress values.

Declaration.

The researcher thanks Sumer University/College of Basic Education/Department of Science for a supportive academic environment conducive to the process of conducting this research. The researcher also recognizes the scientific contributions of the research community in the fields of two-dimensional magnetic materials and computational condensed matter physics that underlie the building of a considerable knowledge base for this work.

Conflict of Interest

The researcher asserts that there are no conflicts of interest in this study.

Conclusion

The paper concluded that two-dimensional magnetic materials were one of the most effective platforms of researching emerging quantum phases in low-dimensional fields, and of developing advanced spintronic and quantum systems. The investigation revealed CrI3 monolayer's intrinsic ferromagnetism at a Curie temperature of 45 K, which was considered that with enough intrinsic magnetic anisotropy to stabilize the system, longer range magnetic ordering exists at two dimensions. Moreover, the engineering of stability in the case of magnetism, mechanical strain can indeed enhance magnetic anisotropy energy through a significant shift, with an observed enhancement in the magnetic anisotropy energy in CrI3 of 47% at 5% stress which illustrates that the structural deformation is also the vital parameter in the engineering of the magnetic stability. Based on the experimental results, the performance of the three different cell doping approaches was demonstrated, with the increase in electron doping not only making the magnetic exchange much better, but also raising the Curie temperature, evidenced in Cr2Ge2Te6 with 0.3 electron doping, where the exchange constant increased from 6.874 meV to 10.202 meV and the Curie temperature rising from approximately 85 K to approximately 123 K (Hou et al., 2023). Combining theoretical mechanical strain and electronic doping, these data support the claim that combining them in a computational framework based on DFT, XXZ-Heisenberg model and Monte Carlo simulation is a sound scientific path

towards exploring new quantum phases and highlighting the best windows for both heating and enhancing the two-dimensional materials magnetic and thermal stability (Kong, et al., 2024). In this way, thus providing an important theoretical and methodological basis for a more comprehensive, computational design of the present computational study to further strengthen its presence in computational condensed matter physics and contemporary functional materials in the literature on this research direction.

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