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The Effect of External Electric Field on The Electrical and Magnetic Properties of $NiCl_2$ Monolayer with Density Functional Theory

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Abstract

The study utilized density functional theory (DFT) to investigate the impact of spin-orbit interaction and external electric fields on the $NiCl_2$ monolayer. The results demonstrated a reduction in the energy band gap and a transition from an indirect semiconductor to a metal when different electric fields were applied. Additionally, the combination of external electric fields and spin-orbit interactions altered the band structure of the $NiCl_2$ monolayer, leading to a transition from a semiconducting state to a metallic state. These findings have significant implications for spintronic device design, as they suggest the potential for controlling the electrical and magnetic properties of the $NiCl_2$ monolayer, making it suitable for use in alternative spintronic devices.

Keywords: $NiCl_2$ monolayer, density functional theory, spin-orbit interaction, external electric field, spintronics

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INTRODUCTION

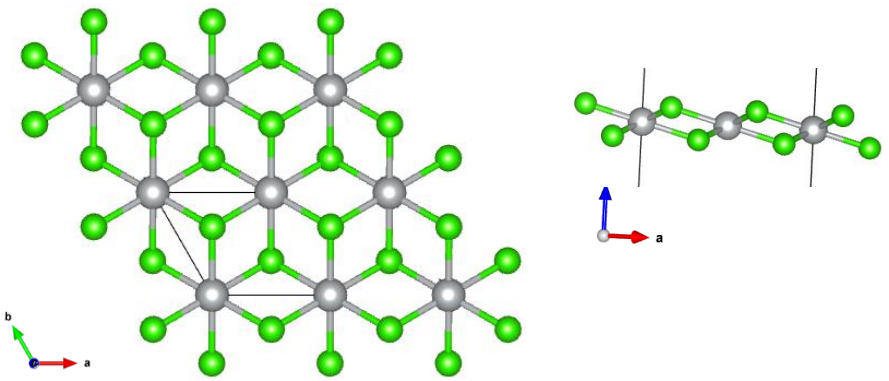
The demand for spintronic devices has grown significantly due to the various applications of spin-orbit interaction (SOI) (Machon et al., 2015). In addition, modifying the material properties by applying an external electric field have also attracted attention. Among the materials that have attracted significant interest in spintronic device development is two-dimensional graphene (Novoselov et al., 2005). Researchers have shown interest in 2D materials like graphene for spintronic device development. Transition Metal Dichalcogenides (TMDCs), especially monolayers like MoX_2 (Manzeli et al., 2017) and WX_2 (where X = S, Se) (Affandi et al., 2018; Affandi et al., 2019). Within TMDCs have been extensively studied for their favorable electronic properties.

The transition metal dihalides (TMD) family of materials possesses similar characteristics, including electronic and magnetic properties. Certain transition metal dichalcogenides (TMDCs) exhibit both a multiferroic properties and a helimagnetic state in their volumetric configurations (Tokunaga et al., 2011; Kurumaji et al., 2013). The efficient synthesis methods for 2D materials have highlighted the importance of studying TMDC monolayers (Kulish et al., 2017).

The primary objective of this study is to investigate the impact of an external electric field and spin-orbit interaction on the electrical and magnetic characteristics of $NiCl_2$ monolayers, which belong to the TMDC family. The results of our research indicate that the application of an external electric field leads to a reduction in both the band gap and magnetic moment of $NiCl_2$ monolayers. The following part will examine the arrangement of $NiCl_2$ monolayers and the computational techniques employed for analysis. Subsequently, we present and discuss the results, utilizing data and ideas from previous studies. Finally, we conclude the study by summarizing our findings and providing concluding remarks.

METHOD

The unit cell of the 1T-$NiCl_2$ monolayer crystal structure consists of one Ni atom and two Cl atoms, as depicted in Figure 1. To accommodate the $NiCl_2$ monolayer, a vacuum space of 17 Å was created, with a lattice parameter of 3.7 Å (Mcguire et al., 2017). The DFT calculations were performed using the OpenMX software (Ozaki et al., 2023), utilizing the generalized gradient approximation (GGA) for the exchange-correlation functionality, including spin-orbit coupling (Perdew et al., 1996). A sampling of the primitive cells was conducted in the first Brillouin zone using a 16 × 16 ×1 *k*-point grid, and a cut energy of 300 Ry was applied.



(a) (b)

Figure 1. The illustration of the crystal structure of the $NiCl_2$ monolayer, providing both a side view (a) and a top view (b) (Silver: Ni and Green: Cl).

For the Ni atom, we utilized the pseudopotential Ni6.0S-s3p3d2f1, which includes a cutoff radius of 6.0 Bohr and incorporates 45 linear combinations of three *s* primitive orbitals, three *p* primitive orbitals, two *d* primitive orbitals, and one *f* primitive orbital. As for the Cl atom, we

employed the Cl7.0-s3p3d2 pseudopotential, featuring a cutoff radius of 7.0 Bohr and Consisting of a total of 22 linear combinations derived from three for each *s* and *p* primitive orbitals and two *d* primitive orbitals, our calculations involved conducting a geometry optimization process to achieve atomic position relaxation in a non-magnetic structure before the analysis, ensuring that the forces applied to the atoms were below 5 × 10-3 eV/Å. Subsequently, we prepared various conditions of external electric fields ranging from 0 to 3.0 V/Å in the positive *z*-axis direction.

RESULTS AND DISCUSSION

In Figure 2, we present the band structure of the $NiCl_2$ monolayer, in both scenarios, considering the presence or absence of spin-orbit interaction. Our calculations revealed that the $NiCl_2$ monolayer exhibits an indirect band gap with semiconductor characteristic, in the state, a conduction band minimum (CBM) is positioned between the M and Γ points, and a the valence band maximum (VBM) at the Γ point. The energy band gaps determined through calculations, considering both cases of with and without spin-orbit interactions, are found to be 1.052 eV and 1.047 eV, respectively. While the band gaps are similar, there is a slight difference in their values, although it is not significant. These band gap values align well with previous calculations, indicating a reasonable agreement while reducing the energy gap. Additionally, the calculated The magnetic strength of the nickel (Ni) atom within the $NiCl_2$ monolayer, both without and with spin-orbit interactions, is found to be 1.426 μ_B and 1.423 μ_B, respectively, within the unit cell.

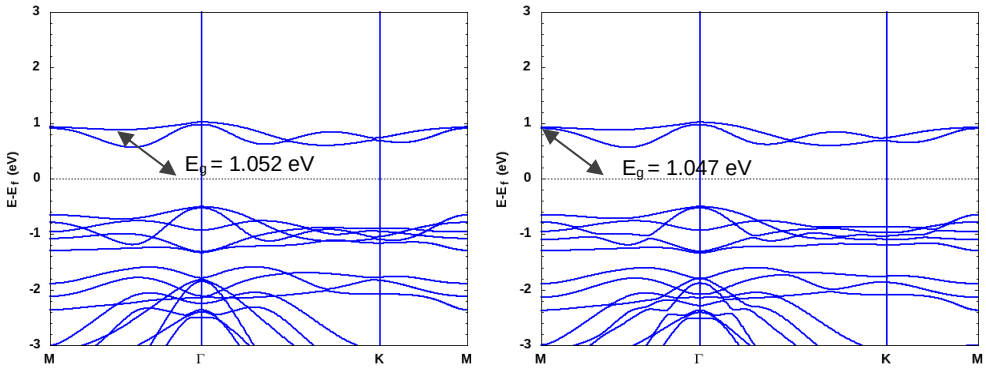


Figure 2. Presents the band dispersions of the $NiCl_2$ monolayer, showcasing the variation in (a) the absence and (b) the inclusion of spin-orbit interaction.

Subsequently, we investigated the outcome of employing an external electric field on the $NiCl_2$ monolayer. The results, as depicted in Figure 3, demonstrate that The combination of the external electric field and spin-orbit interactions being present alters the band structures of the $NiCl_2$ monolayer, causing a transition from a semiconductor state to a metallic state. As the magnitude of the applied electric field increases, the $NiCl_2$ state transforms into a metallic state. In Figure 4, we compare the values of the external electric field with the band gap energy and magnetic moment of the Ni atom after incorporating these effects. Remarkably, with the increasing magnitude of the external electric field, There is a decrease in the energy of the band gap. accompanied by a significant change in the magnetic moment of the Ni atom. These changes occur gradually until both

magnitudes eventually reach zero. However, it is noteworthy that the magnetic moment of Ni reemerges when the external electric field reaches a magnitude of 3 V/Å, in conjunction with the spin-orbit interaction effect. This finding holds significance for spintronic applications, This indicates the transformation of the electrical characteristics in the $NiCl_2$ monolayer, shifting from being an indirect band gap semiconductor to acquiring metallic properties.

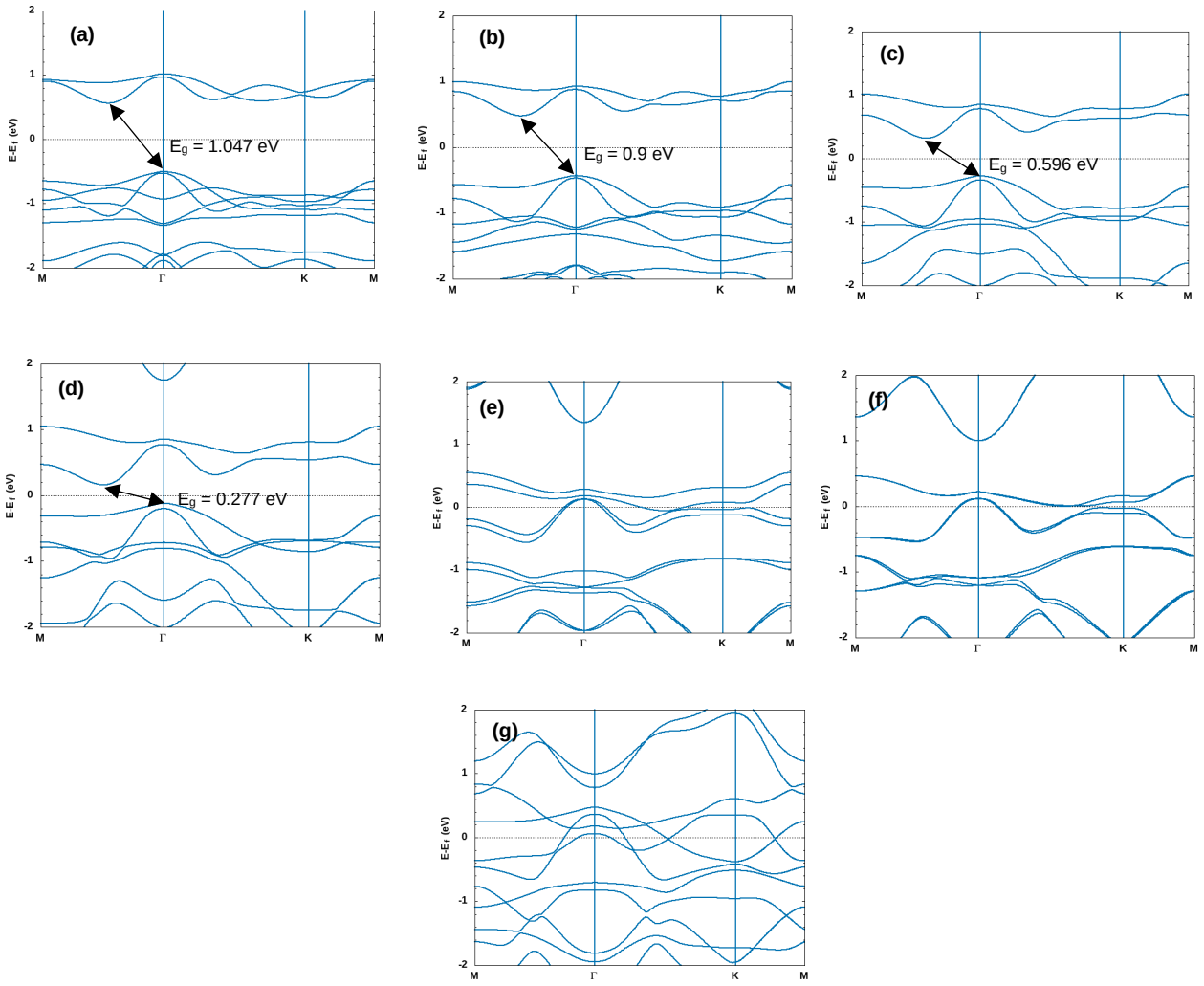


Figure 3. Illustrates the band structures of the $NiCl_2$ when subjected SOI through different electric field strengths, specifically (a) 0.0 V/Å, (b) 0.5 V/Å, (c) 1.0 V/Å, (d) 1.5 V/Å, (e) 2.0 V/Å, (f) 2.5 V/Å, and (g) 3.0 V/Å.

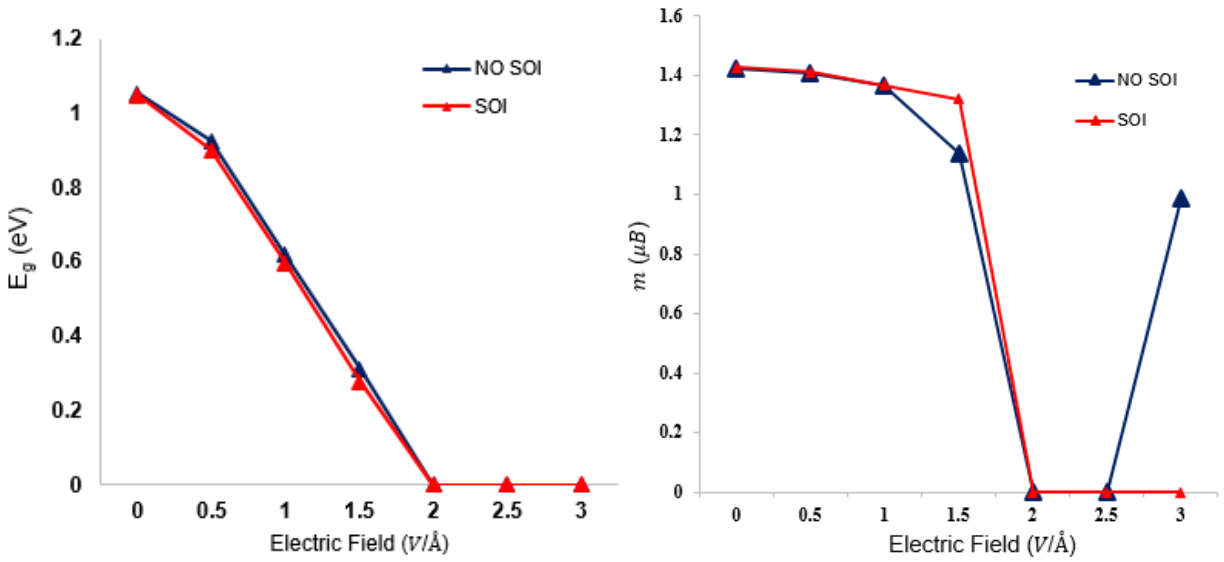


Figure 4. The variatioin in (a), the energy gap, and in (b), the magnetic moimeint of the nickel (Ni) atom within the $NiCl_2$ monolayer, as influenced by an external electric field. The data presented in the figure accounts for both the scearios without and with the inclusion of spin-orbit interaction.

In our research on the transition of the band gap, an intriguing discovery was made regarding spin-splitting. This phenomenon was observed in the conduction band at Γ point and valence band between the Γ and K points, with energy splitting of 113 meV and 117 meV, respectively. This spin-splitting arises from the presence of broken spatial inversion symmetry in the monolayer structure, resulting in a slight separation of energy bands. In comparison to the findings of a previous study (Manzeli et al., 2017), the energy splitting observed in our research is relatively narrow, suggesting the potential for enhanced electrical field effects and the generation of significant energies. The manifestation of spin-splitting in the $NiCl_2$ monolayer highlights its promising suitability for spintronic applications.

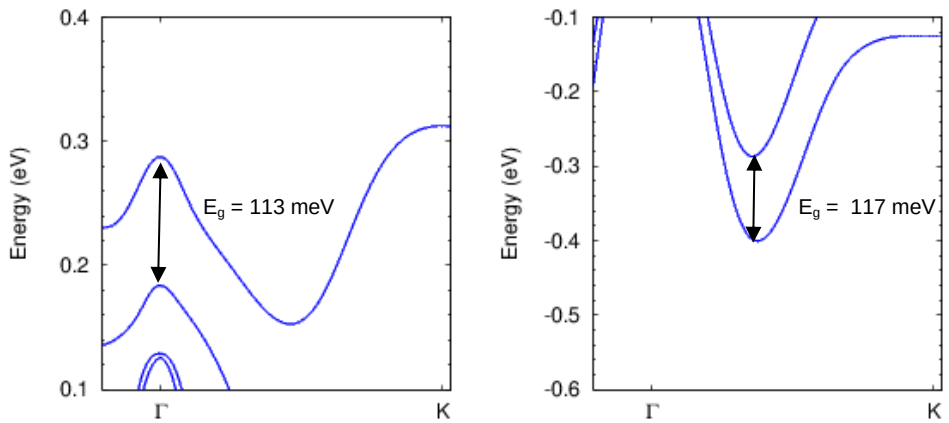


Figure 5. Energy that indicates spin-splitting in (a) conduction band and (b) valence band for Ni monolayer when an electric field oif 2 V/Å is applied and combined with the effect of spin orbit $NiCl_2$ interaction.

CONCLUSION

Based on our exploration, it is evident that the interaction between spin and orbit, when combined with an external electric field, has a noticeable but not significant impact on the energy band of $NiCl_2$ monolayers. This interaction affects both the energy gap and magnetic moment of nickel atoms. Significantly, it transforms the $NiCl_2$ monolayer from a semiconductor with an indirect band gap to a metallic state, accompanied by the occurrence of spin splitting. This study emphasizes the manipulability of the electrical and magnetic characteristics of $NiCl_2$ monolayers through the application of external electric fields. These discoveries are crucial for the progress of thermoelectric materials and will provide guidance for future investigations in this field.

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