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Structural and Electronic Properties of Janus Sc_2CBT (T = H, F) MXenes

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ABSTRACT

In this study, Sc_2CBT (T=H, F) Janus MXene monolayers have been investigated for the first time using density functional theory calculations. The lattice constants, bond lengths, cohesive energies, magnetic properties, and electronic properties have been examined in detail. The obtained findings have shown that Sc_2CBF Janus MXene monolayer is energetically stable. The calculations showed that none of the monolayers exhibits magnetic ordering. The electronic band structure calculations have demonstrated that both monolayers exhibit metallic character. Additionally, it was understood that the boron element significantly affects the electronic properties of both monolayers. This study is the first to investigate Sc_2CBH and Sc_2CBF Janus monolayers, and the findings are discussed in detail.

1. Introduction

Two-dimensional (2D) MXenes [1, 2] have extraordinary properties due to their unique properties such as supercapacitors [3], sensing devices [4], electronics [5, 6], photo-catalysis and solar cell applications [7]. A novel subclass of MXenes, known as Janus MXenes, has emerged, featuring an asymmetrical surface termination that imparts unique properties not found in their symmetrical counterparts. Janus MXenes are characterized by their dual nature, where each side of the monolayer is terminated with different atoms, resulting in broken mirror symmetry, and inducing out-of-plane dipolar polarization [8, 9]. This asymmetry has been shown to significantly alter electronic structures, making Janus MXenes promising candidates for applications in various electronic devices.

MXene compounds are synthesized by removing the A element from MAX compounds, and as a result, their surfaces are inevitably functionalized with different groups due to the complex chemical process. Depending on the chemical process, their surfaces can generally be functionalized with O, H, F, OH, or other terminal groups. These surface terminal groups can directly affect the structural, electronic, optical, magnetic, or transport properties of MXene compounds. The Sc_2CT_2 (T = O, F, OH, B, Cl, etc.) pure MXene compound is obtained by removing the Al element from the Sc_2AlC MAX compound. During this process, its surface can be terminated with F, Cl, Br, O, H, B, or other similar terminal groups [10], and its structural and electronic properties are influenced by these groups. Although the precursor to the Sc_2C MXene compound, the Sc_2AlC AX compound, has been chemically synthesized [11], the structural and electronic properties of the Sc_2CBF and Sc_2CBH Janus MXene compounds have not yet been investigated. However, Sc_2C-based Janus MXenes also have been the subject of several studies, focusing on their unique structural and electronic properties, as well as their potential applications in various advanced technologies [12-14]. Liu et al. [15] conducted a theoretical exploration of the potential applications of Sc-based MXenes, including Janus MXenes. The study highlighted their potential use in field-effect transistors, spintronics, optoelectronics, solar energy conversion, and photocatalysis, demonstrating the broad applicability of these materials in advanced technological applications [15]. Furthermore, recently, Cui et al. [18] studied electronic, optical, and photocatalytic and quantum capacitance of ScC_2T_2 (T= F, P, Cl, Se, Br, O, Si, S, OH) MXenes. In addition, very recently, Modi et al. [17] confirmed structural stability and investigated pressure-driven electronic, and optical properties of Sc_2CBr_2 MXene. The electronic properties of Sc_2XT, (X = O, F, OH; T= C, S, N) Janus MXenes were investigated using density functional theory by Ozcan et el. [18] and they found that these materials to be semiconductors with suitable bandgaps for nano and optoelectronics applications. Another study on Sc-based Janus MXenes was recently conducted by Zhu et al. [19] and Sc_2COHH, Sc_2COHF, Sc_2OHCl, Sc_2CHF, Sc_2CHCl, and Sc_2CFCl Janus MXenes were examined in terms of nanoelectromechanical applications.

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In addition to the fact that 2D structures remain a very important research topic, this study is significant because the surface of the Sc_2CT MXene compound is terminated asymmetrically with different atoms, and its electronic structure is primarily examined based on the Boron (B) element. In this paper, extending the understanding of Janus MXenes was aimed by focusing on the less explored Sc_2C and B based compounds. By employing Density Functional Theory (DFT) calculations, the structural and electronic properties, and potential applications of boron based Sc_2CBH, and Sc_2CBF Janus MXenes were analyzed for the first time. These insights will contribute to the growing body of knowledge on Janus MXenes and their applicability in future technological innovations.

2. Computational Methods

Spanish Initiative for Electronic Simulations with Thousands of Atoms (SIESTA) [20, 21] is a method and its software implementation designed for electronic structure calculations and ab initio molecular dynamics simulations, utilizing atomic orbitals as a basis set. First-principles calculations were performed using the SIESTA code with split-type double zeta polarized (DZP) [22] atomic orbitals basis sets. These calculations employed spin-polarized Perdew-Burke-Ernzerhof (PBE) [23] exchange-correlation functionals under the Generalized Gradient Approximation (GGA), revPBE [24] exchange correlation functionals under the (GGA), CA [25] under the Local Density Approximation (LDA) and van der Waals (vdW-DF) with BH functional [26]. The conjugate gradient (CG) method [27] was used for relaxation, and all atoms were fully relaxed until the forces on each atom were lower than 0.01 eV/Å. An energy cutoff of 300 Ry was set, and a 30×30×1 Monkhorst-Pack [28] k-point sampling was used for relaxation and electronic structure calculations. Electron-ion interactions were addressed using non-relativistic Troullier-Martin norm-conserving pseudopotentials [29]. To prevent interaction between repeating layers, over 15 Å of vacuum was applied in the z-direction. The electronic band structure calculation was performed along the Γ-M-K-Γ high symmetry points in Brillouin Zone (BZ). A standard orbital-confining cutoff energy of 100 meV was used in all calculations. Further analysis of structural stability such as cohesive energies was calculated using Equ. 1 [17].

$$E_{cohesive} = \frac{[E_{total}(Sc_2CBT - 2E(Sc) - E(C) - E(B) - E(T)}{5} \qquad (1)$$

In Equation 1, E_{total} represents the total energy of Sc_2CBT Janus monolayer, *E(Sc)*, *E(B)*, and *E(T)*, represents total energy of Sc atom, B atom and T= (B, F) atoms respectively.

3. Results and Discussion

The 2D Sc_2CBT MXene compound belongs to space group number 164, trigonal structure (Figure 1). The calculations were made on with a 1×1×1 unit-cell containing 2 Sc atoms, 1 C atom, 1 B atom and 1 T = (H, F) surface termination atom.

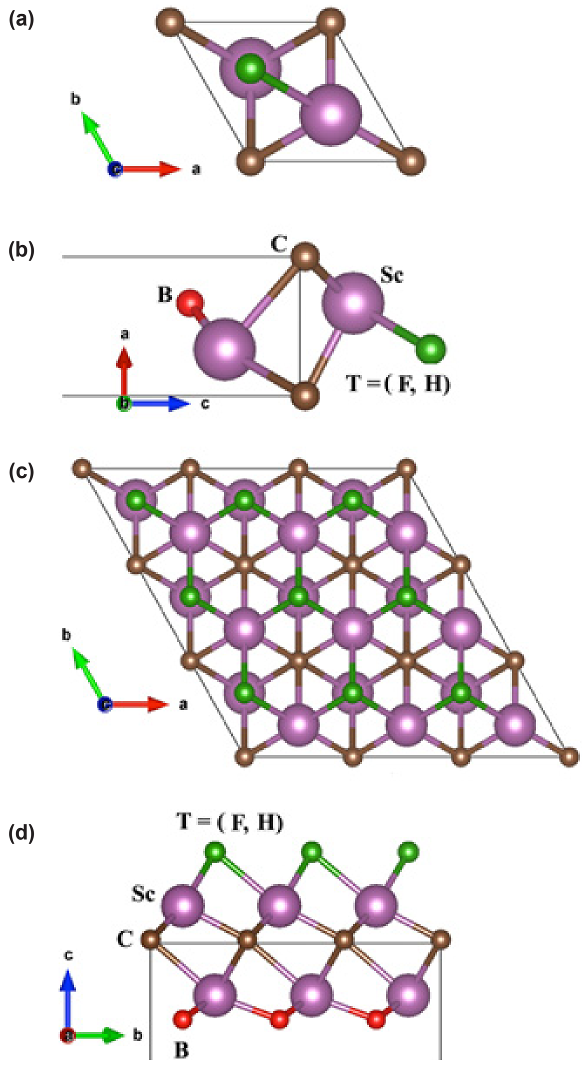

Figure 1. a) Top view of the unitcell of the monolayer Sc_2CBT, b) Side view of the unitcell Sc_2CBT, c) Top view of the 3×3×1 supercell Sc_2CBT, d) Side view of the 3×3×1 supercell Sc_2CBT. The Sc, C, B, and T atoms represent purple, brown, red, and green colors, respectively..

Previous studies [14, 15] on the same structure have stated that the most suitable position for the atoms to be placed for surface termination is top of the Sc atoms. For this reason, in this study, H and F atoms were placed top of the Sc atoms. Firstly, the magnetic nature of the Sc_2CBH compound were investigated. In this study, spin-polarized, ferromagnetic (FM), antiferromagnetic (AFM), and non-spin-polarized (NM) calculations were performed to determine the lattice parameters and total energies. No net magnetic moment was observed in any of the calculations. Furthermore, no difference in energy was observed between each magnetic ordering for Sc_2CBH and Sc_2CBF monolayers. Only for Sc_2CBH, the energy for the AFM state was slightly lower but there was no significant difference. This means that the compounds Sc_2CBH and Sc_2CBF monolayers do not possess any magnetic nature. Since no difference was observed for the magnetic ordering, structural calculations were continued using different exchange-correlation functions for FM ordering. The results of these calculations are presented in Table 1.

Table 1. Calculated total energies (in eV), and lattice parameters (in Å) for Sc_2CBH and Sc_2CBF Janus monolayers with, PBE, revPBE, VDW-BH and LDA exchange-correlation functionals.

Compound	Sc_2CBH		Sc_2CBF	
	Lattice Constant (Å)	Total Energy (eV)	Lattice constant (Å)	Total Energy (eV)
PBE	3.30	-407.69	3.29	-1063.72
revPBE	3.31	-408.25	3.30	-1064.75
VDW-BH	3.29	-407.51	3.28	-1063.07
LDA	3.28	-404.39	3.26	-1057.58

As seen in Table 1, in both structures, revPBE has the lowest energy, which could be explained by the Lieb-Oxford (LO) bound [30]. In a non-spin-polarized system, revPBE is sufficient to identify LO bounds, but in a spin-polarized system, there is no guarantee [28]. The VDW-BH exchange-correlation functional also includes weaker forces, and these weak forces result in smaller lattice parameters. LDA has the highest energy, indicating that a local electron distribution does not adequately describe the system in these structures. Furthermore, as seen in both structures, higher lattice parameters were obtained with revPBE exchange-correlation functionals. When evaluated in general, it is observed that the use of different exchange-correlation functionals causes a difference of approximately 0.6% in the lattice parameters of Sc_2CBF and Sc_2CBH compounds. In addition, the difference in total energy between revPBE and PBE exchange-correlation functionals is negligibly low. In this case, the calculations were continued with the PBE exchange-correlation functional. The bond lengths and calculated cohesive energies, along with the lattice parameters, are presented in Table 2.

Table 2. Calculated lattice constants (in Å), distance between Sc-B atoms, dSc-B (in Å) and distance between Sc-T (T = H, F) atoms dSc-T (in Å) and cohesive energies $E_{cohesive}$ (in eV/atom) for Sc_2CBH and Sc_2CBF Janus monolayers.s.

Compound	Lattice Constant (Å)	d_{Sc-B} (Å)	d_{Sc-T} (Å)	$E_{Cohesive}$ (eV/atom)
Sc_2CBH	3.30	2.48	2.17	0.28
Sc_2CBF	3.29	2.51	2.24	-0.70

In Table 2, lattice constants were calculated 3.30 Å for Sc_2CBH and 3.29 Å for Sc_2CBF from PBE exchange-correlation function. The dSc-B bond length is the same in both compounds 2.48 Å, suggesting a similar bonding environment for Sc and B atoms in these structures. The slight difference in the dSc-T bond lengths between Sc_2CBH and Sc_2CBF are 2.17 Å, and 2.24 Å, respectively. This can be attributed to the different nature of the terminal atoms since H, being smaller, forms a shorter bond with Sc compared to F. Although the structural parameters are similar, the differences in dSc-T bond lengths could lead to variations in physical properties such as bond strength, electronic properties, and chemical reactivity between the two compounds. The structural stability of Sc_2CBr_2 and Sc_2CT_2 (T= F, P, Cl, Se, Br, O, Si S, OH) MXenes confirmed with previous studies [16, 17]. However, Sc_2CBH and Sc_2CBF also investigated first time and therefore, cohesive energies were calculated. As can be seen from Table 2, the cohesive energies of Sc_2CBH and Sc_2CBF Janus monolayers are 0.28 eV/atom and -0.70 eV/atom respectively. Negative cohesive energy values indicate that significant energy is required to remove T atoms from the system, predicting energetical stability. The Janus Sc_2CBF is energetically stable due to its negative cohesive energy. In contrast, the compound Sc_2CBH could not be stable because it possesses a positive cohesive energy, although very low, which may imply metastability for the Janus Sc_2CBH monolayer. Furthermore, the cohesive energy value for H being higher than that for F atoms with the observation that the bond length between Sc and H is shorter than that between Sc and F. The low cohesive energy of the Sc_2CBF compound makes it a suitable candidate for specific applications, such as temporary electronic devices or reconfigurable circuits [31]. This property also allows the material to break down easily, making it useful in controlled release systems like drug delivery [32].

After confirming structural stability, electronic properties were investigated. The calculated electronic band structure of Sc_2cBH and Sc_2CBF Janus monolayers are presented in Figure 2.

Figure 2 shows the electronic band structures of Sc_2CBH and Sc_2CBF Janus monolayers. The band structure of Sc_2CBH Janus monolayer reveals multiple bands intersecting the Fermi level, indicative of metallic behavior. Like Sc_2CBH, Sc_2CBF also shows multiple bands crossing the Fermi level, indicating metallic properties as well. Moreover, the band branches passing the Fermi level within each Janus MXene are plotted in blue and red color, unlike other bands. As can be seen, these two band branches in both structures give the structures a metallic character. To better examine their electronic properties, the partial density of states (PDOS) has been calculated. The PDOS of Sc_2CBH Janus MXene is presented in Figure 3.

In Figure 3, the Fermi level is set to E=0 eV. Although the dominant contribution to the PDOS in the Sc_2CBH monolayer comes from Sc atoms, near the Fermi level, most of the contribution comes from B atoms. This situation indicates that the electronic properties of the Janus Sc_2CBH monolayer are mainly determined by

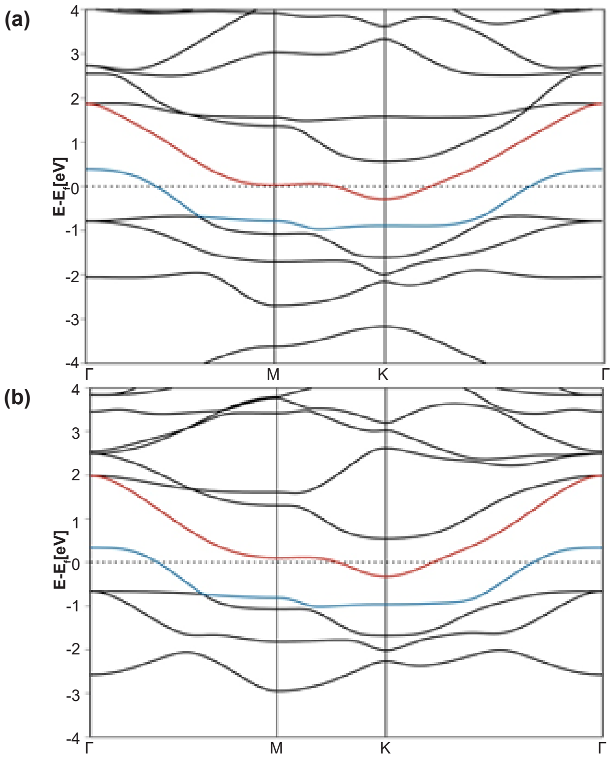

Figure 2. Electronic band structure of Sc_2CBT (T= H, F) monolayers a) Sc_2CBH Janus MXene, b) Sc_2CBF Janus MXene.

the B atoms. There are significant peaks near -1.0 eV and 1.5 eV, indicating strong participation of Sc atoms in the electronic states near the Fermi level. The C atoms contribute states primarily below the Fermi level, indicating that their states are mostly filled and do not play a significant role in the conduction properties. H atoms show very low contributions across the energy range, indicating a minimal impact on the electronic structure.

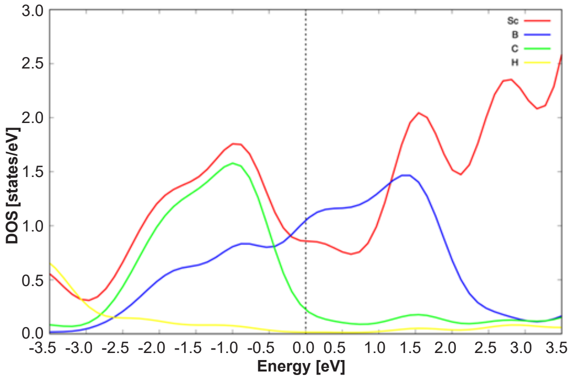

Figure 3. PDOS of Sc_2CBH Janus MXene.

For further analysis, PDOS of Sc_2CBF compound was calculated and it is presented in Figure 4.

As seen in Figure 4, similar to Sc_2CBH, although Sc atoms generally appear dominant, B atoms are still the most dominant at and around the Fermi level. Even though the surface termination element changes, B atoms maintain their dominance. Although the Sc_2CBF compound exhibits a pattern similar to that of the Sc_2CBH compound, a noticeable change in the distribution of Sc atoms is evident, especially in the positive energy region. This distribution of states is due to the presence of the F atom. The contribution from carbon is again mostly below the Fermi level, similar to the Sc_2CBH monolayer. F atoms show very minimal contribution to the PDOS across the energy range, like H in the Sc_2CBH monolayer. This suggests that fluorine's impact on the electronic structure is minimal.

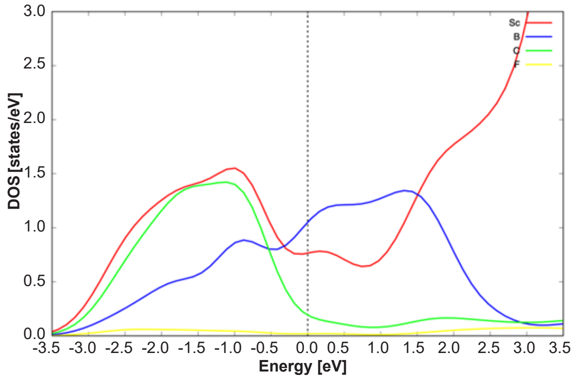

Figure 4. PDOS of Sc_2CBF Janus MXene.

Both monolayers exhibit significant contributions from Sc and B near the Fermi level, suggesting that these elements are primarily responsible for the electronic properties of these materials. The presence of H in Sc_2CBH and fluorine in Sc_2CBF does not significantly alter the overall PDOS, indicating that these atoms have a minor role in the electronic properties. The peaks just below and above the Fermi level are indicative of the potential for these materials to exhibit interesting electronic properties, such as metallic behavior or specific conductive properties.

4. Conclusions

Sc_2CBH and Sc_2CBF Janus MXene monolayers have been studied for the first time for their structural, magnetic, and electronic properties using DFT calculations. The stability of Janus Sc_2CBF monolayer has been confirmed by the cohesive energy. Moreover, electronic band structure calculations showed their metallic nature. Computational analyses of AFM and ferromagnetic FM states indicate that the Sc_2CBH and Sc_2CBF compounds do not exhibit magnetic properties. Although the lowest energy was obtained with revPBE through relaxation calculations using different exchange-correlation functionals, the difference compared to the PBE exchange-correlation functional is insignificant. When examining the electronic properties, it is observed that while Sc atoms generally appear dominant, B atoms, which are predominant at the Fermi level, have a direct effect on the electronic properties. This is an important result for boron and Sc based MXenes. Moreover, although the PDOS of F and H atoms in both compounds does not have a significant impact on the electronic properties as expected, it is observed that Sc atoms influence the distribution in the positive energy region.

Sc_2CBF has been understood to have potential applications in temporary electronic devices, reconfigurable circuits, controlled drug release. The findings obtained in this study will be used for future experimental and theoretical studies on B and Sc based Sc_2CBT Janus MXenes.

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References

[1] Naguib, M., Kurtoglu, M., Presser, V., Lu, J., Niu, J., Heon, M., ... & Barsoum, M.W. (2011). Two-dimensional nanocrystals produced by exfoliation of Ti3AlC2. *Advanced Materials*, *23*(37), 4248-4253. https://doi.org/10.1002/adma.201102306

[2] Naguib, M., Mochalin, V. N., Barsoum, M. W., & Gogotsi, Y. (2013). 25th anniversary article: MXenes: A new family of two-dimensional materials. *Advanced Materials*, *26*(7), 992-1005. https://doi.org/10.1002/adma.201304138

[3] Ghidiu, M., Lukatskaya, M. R., Zhao, M. Q., Gogotsi, Y., & Barsoum, M. W. (2014). Conductive two-dimensional titanium carbide 'clay' with high volumetric capacitance. *Nature*, *516*, 78-81. https://doi.org/10.1038/nature13970

[4] Yu, X. F., Li, Y.C., Cheng, J. B., Liu, Z. B., Li, Q. Z., Li, W. Z., Yang, X., & Xiao, B. (2015). Monolayer Ti2CO2: A promising candidate for NH3 sensor or capturer with high sensitivity and selectivity. *ACS Applied Materials & Interfaces*, *7*(24), 13707-13713. https://doi.org/10.1021/acsami.5b03737

[5] Khazaei, M., Ranjbar, A., Ghorbani-Asl, M., Arai, M., Sasaki, T., Liang, Y., & Yunoki, S. (2016). Nearly free electron states in MXenes. *Physical Review B*, *93*(20), 205125. https://doi.org/10.1103/PhysRevB.93.205125

[6] Feng, L., Zha, X. H., Luo, K., Huang, Q., He, J., Liu, Y., ... & Du, S. (2017). Structures and mechanical and electronic properties of the Ti2CO2 MXene incorporated with neighboring elements (Sc, V, B and N), *Journal of Electronic Materials*, *46*(4), 2460-2466. https://doi.org/10.1007/s11664-017-5311-5

[7] Zhang, Y., Sa, B., Miao, N., Zhou, J., & Sun, Z. (2021). Computational mining of Janus Sc2C-based MXenes for spintronic, photocatalytic, and solar cell applications. *Journal of Material Chemistry A*, *9*(17), 10882-10892. https://doi.org/10.1039/D1TA00614B

[8] Xiong, K., Cheng, Z., Liu, J., Liu, P. F., & Zi, Z. (2023). Computational studies on functionalized Janus MXenes MM'CT2, (M, M' = Zr, Ti, Hf, M ≠ M'; T = -O, -F, -OH): Photoelectronic properties and potential photocatalytic activities. *RSC Advances*, *13*(12), 7972-7979. https://doi.org/10.1039/D3RA00303E

[9] Murari, H., & Ghosh, S. (2024). Symmetry lowering through surface engineering and improved thermoelectric properties in Janus MXenes. *Nanoscale*, *16*(23), 11336-11349. https://doi.org/10.1039/D4NR00568F

[10] Natu, V., & Barsoum, M. W. (2023). MXene surface terminations: A perspective. *Journal of Physical Chemistry C*, *127*(41), 20197-20206. https://doi.org/10.1021/acs.jpcc.3c04324

[11] Ali, M. A., Nasir, M. T., Khatun, M. R., Islam, A. K. M. A., & Naqib, S. H. (2016). An ab initio investigation of vibrational, thermodynamic, and optical properties of Sc2AlC MAX compound. *Chinese Physics B*, *25*(10), 103102. http://doi.org/10.1088/1674-1056/25/10/103102

[12] Lv, X., Wei, W., Sun, Q., Lin, Y., Huang, B., & Dai, Y. (2017). Sc2C as a promising anode material with high mobility and capacity: A first-principles study. *ChemPhysChem*, *18*(12), 1627-1634. https://doi.org/10.1002/cphc.201700181

[13] Hu, Q., Wang, H., Wu, Q., Ye, X., Zhou, A., Sun, D., ... & He, J. (2014). Two-dimensional Sc2C: A reversible and high-capacity hydrogen storage material predicted by first-principles calculations. *International Journal of Hydrogen Energy*, *39*(20), 10606-10612. https://doi.org/10.1016/j.ijhydene.2014.05.037

[14] Kumar, S., & Schwingenschlögl, U. (2016), Thermoelectric performance of functionalized Sc2C MXenes. *Physical Review B*, *94*(3), 035405. https://doi.org/10.1103/PhysRevB.94.035405

[15] Liu, J. H., Kan, X., Amin, B., Gan, L. Y., & Zhao, Y. (2017). Theoretical explanation of the potential applications of Sc-based MXenes. *Physical Chemistry Chemical Physics*, *19*(48), 32253-32261. https://doi.org/10.1039/C7CP06224A

[16] Cui, X. H., Li, X. H., Zhang R. Z., Cui, H. L., & Yan, H. T. (2023). Theoretical insight into the electronic, optical, and photocatalytic properties and quantum capacitance of Sc2T2 (T = F, P, Cl, Se, Br, O, Si, S, OH) MXenes. *Vacuum*, *207*, 111615. https://doi.org/10.1016/j.vacuum.2022.111615

[17] Modi, N., Naik, Y., Khengar, S. J., Shah, D. B., & Thakor, P. B. (2024). Pressure induced structural, electronic, and optical properties of Sc2CBr2 MXene monolayer: A density functional approach. *Computational and Theoretical Chemistry*, *1232*, 114466. https://doi.org/10.1016/j.comptc.2024.114466

[18] Ozcan, S., & Biel, B. (2023). Exploring a novel class of Janus MXenes by first principles calculations: Structural, electronic, and magnetic properties of Sc2CXT, X = O, F, OH; T=C, S, N. *Physical Chemistry Chemical Physics*, *25*(3), 1881-1888. https://doi.org/10.1039/d2cp04713f

[19] Zhu, S. Y., Li, Y. Q., Wang, X. Y., Tang, D. S., He, Q. W., Liu, C., ... & Wang X. C. (2023). Theoretical investigations of Sc2C based functionalized MXenes for applications in nanoelectromechanical systems. *Physica E: Low Dimensional Systems and Nanostructures*, *145*, 115491. https://doi.org/10.1016/j.physe.2022.115491

[20] Soler, J. M., Artacho, E., Gale, J. D, García, A., Junquera, J., Ordejón, P., & Sanchez-Portal, D. (2002). The SIESTA method for ab initio order-N materials simulation. *Journal of Physics: Condensed Matter*, *14*(11), 2745-2779. https://doi.org/10.1088/0953-8984/14/11/302

[21] Ordejón, P., Artacho, E., & Soler, J. M. (1996). Self-consistent order-N density-functional calculations for

very large systems. *Physical Review B*, *53*(16), 10441-10444. https://doi.org/10.1103/PhysRevB.53.R10441

[22] Junquera, J., Paz, Ó., Sánchez-Portal, D., & Artacho, E. (2001). Numerical atomic orbitals for linear-scaling calculations. *Physical Review B*, *64*(23), 235111. https://doi.org/10.1103/PhysRevB.64.235111

[23] Perdew, J. P., Burke, K., &, Ernzerhof, M. (1996). Generalized gradient approximation made simple. *Physical Review Letters*, *77*(18), 3865. https://doi.org/10.1103/PhysRevLett.77.3865

[24] Zhang, Y., & Yang, W. (1998). Comment on “Generalized gradient approximation made simple”, *Physical Review Letters*, *80*(4), 890. https://doi.org/10.1103/PhysRevLett.80.890

[25] Ceperley, D. M., & Alder B. J. (1980). Ground state of the electron gas by a stochastic method. *Physical Review Letters*, *45*(7), 566-569. https://doi.org/10.1103/PhysRevLett.45.566

[26] Berland, K., & Hyldgaard, P. (2014), Exchange functional that tests the robustness of the plasmon description of the van der Waals density functional. *Physical Review B*, *89*(3), 035412. https://doi.org/10.1103/PhysRevB.89.035412

[27] Hestenes, M. R., & Steiefel, E. (1952). Methods of conjugate gradients for solving linear systems. *Journal of Research of the National Bureau of Standarts*, *49*(6), 409-436. https://doi.org/10.6028/JRES.049.044

[28] Monkhorst, H. J., & Pack, J. D. (1976). Special points for Brillouin-zone integrations. *Physical Review B*, *13*(12), 5188. https://doi.org/10.1103/PhysRevB.13.5188

[29] Troullier, N., & Martins, J. L. (1991). Efficient pseudopotentials for plane-wave calculations. *Physical Review B*, *43*(3), 1993-2006. https://doi.org/10.1103/PhysRevB.43.1993

[30] Vela, A., Medel, V., & Trickey, S. B. (2009). Variable Lieb-Oxford bound satisfaction in a generalized gradient exchange-correlation functional. *Journal of Chemical Physics*, *130*(24), 244103. https://doi.org/10.1063/1.3152713

[31] Hwang, S. W., Tao, H., Kim D. H., Cheng, H., Song, J. K., Rill, E., ... & Rogers J. A. (2012), A physically transient form of silicon electronics. *Science*, *337*(6102), 1640-1644. https://doi.org/10.1126/science.1226325

[32] Zou, R., Li, J., Yang, T., Zhang, Y., Jiao, J., Wong, K. L., & Wang, J. (2021). Biodegradable manganese engineered nanocapsules for tumor-sensitive near-infrared persistent luminescence/magnetic resonance imaging and simultaneous chemotherapy. *Theranostics*, *11*(17), 8448-8463. https://doi.org/10.7150/thno.59840