A First Principle study on structural, electronic and magnetic properties of bilayer T-VSe_2(001)/Co heterostructure

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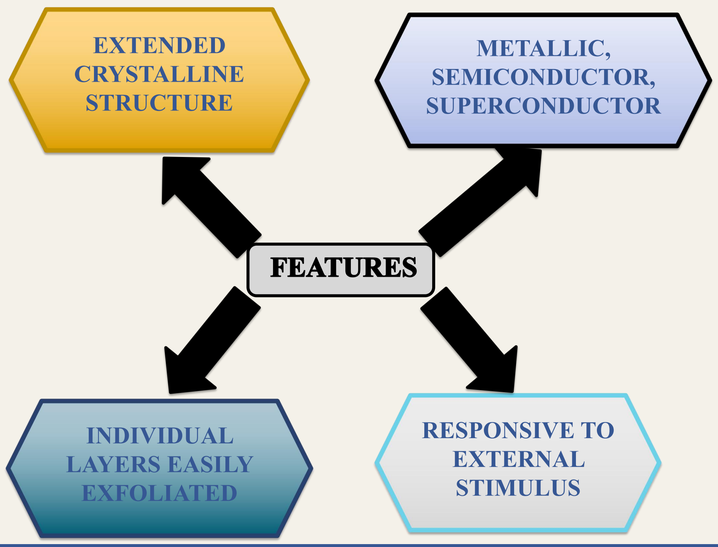
INTRODUCTION

- ✓The discovery of graphene has led to a scientific frenzy in the study of two-dimensional (2D) materials that shows exotic physical properties ultimately leading to real applications.
- ✓Particularly attractive materials are the transition-metal dichalcogenides (TMDs), due to their van der Waals layered structures and their wide range of material properties.
- ✓Controlling the material thickness down to the single-atom scale enables tuning of the interacting electronic states and phases and it is thus highly desirable to fabricate high-quality monolayer (ML) TMDs.
- ✓Vanadium diselenide (VSe_2) is a typical TMD material. The VSe_2 monolayer is composed of metal V atoms sandwiched between two Se atom, and the Se−V−Se layers are stacked in the (001) direction without lateral displacement forming trigonal (T) phase polytype crystal (figure shown) in the bulk.



RESEARCH QUESTION

- ✓What could we do with the layered structures with just the right layers?
- ✓Are these layered materials even applicable in real life?
- ✓Can we tune the properties of such structures by capping it with different material?

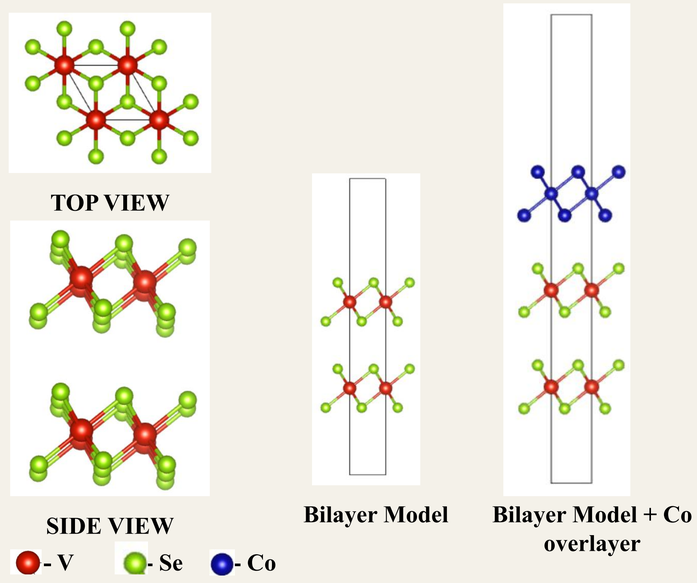
Experimentally, the verification of magnetism in monolayer materials has been hampered by the chemical instability under ambient conditions. In this work, we aim to address these issues by performing density functional theory (DFT) computations.

RESEARCH OBJECTIVES

- ✓Exploring the magnetic properties of vanadium selenium(VSe_2) by increasing the layered structure in succession.
- ✓Check the influence of U parameter and vanderwaal correction on the magnetic moment of these structures.
- ✓Investigating the effect of Co overlayer on the density of states at the Fermi level.
- ✓Exploring the variation of electronic properties on VSe_2 bilayer system

COMPUTATED MODELS

Bulk VSe_2 forms layered crystal (T-phase) with the separate layers stacked along the (001) direction (c-axis direction).



COMPUTATIONAL METHODS

MODELLING	VSe_2(T-phase) was modelled from bulk in various layers
PARAMETERS ADOPTED	On-site U(=3 eV) and Grimme DFT+D3 correction was adopted
ELECTRONIC STRUCTURE CALCULATION	Calculations were done using VASP, within the framework of DFT

RESULTS

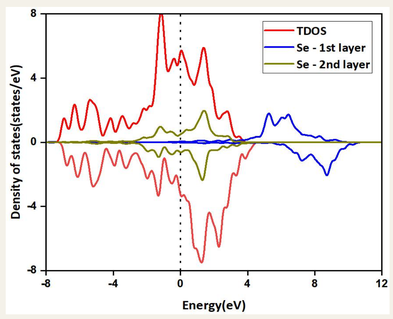


Fig (a) PDOS of VSe_2 without U

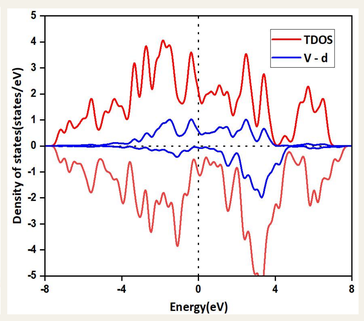


Fig (b) PDOS of VSe_2 with U= 3.0 eV

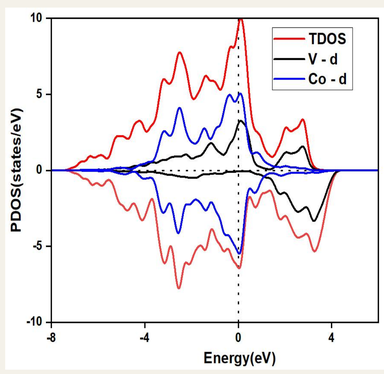


Fig (c) PDOS of T-VSe_2 without vdw

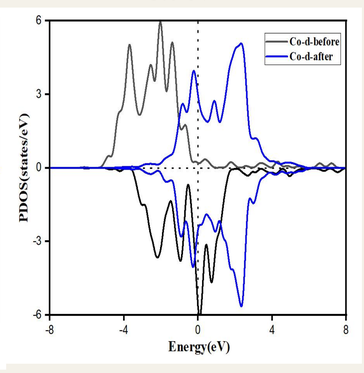


Fig (d) PDOS of Co at VSe_2/Co interface

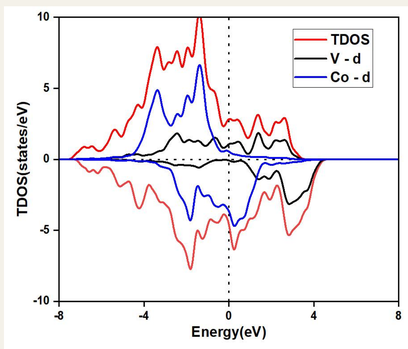


Fig (e) PDOS of T-VSe_2 with vdw

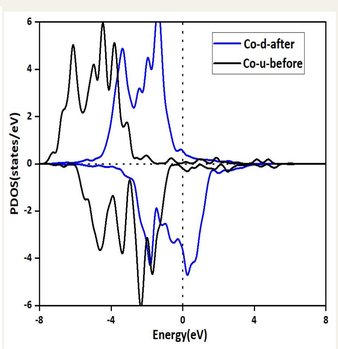


Fig (f) PDOS of Co at VSe_2/Co interface

DISCUSSION

- ✓The total density of states and partial density of states were plotted for bilayer VSe_2 and VSe_2/Co junction and we it was observed that the vdw correction provides more stability to the overall system.
- ✓Without vdw correction, system exhibits ferromagnetism with anti alignment of VSe_2 with Co. However, with correction the overall system shows ferromagnetism.
- ✓The PDOS of 3-ML Co before and after deposition[Fig(d), Fig(f)] shows a shift of the Co spin down band to lower energy and thus a reduction in the exchange splitting. This shows interfacial hybridization between Co and VSe_2 at the interface, leading to a reduction in the Co spin moment.

CONCLUSION

- ✓The structural, magnetic and electronic properties of VSe_2 bilayer and VSe_2/Co vertical junction were studied using DFT+U and vdw correction.
- ✓It was found that the stability of the T phases of VSe_2 monolayers are linked to strong electron correlation effects.
- ✓The magnetic interface of VSe2/Co is free from extrinsic contamination and can be useful in spin based devices and data storage.

IMPLICATIONS

- ✓Integration of various 2D circuit elements into 2D logic and memory circuits could be an attractive way to create ultradense, low-power, flexible electronics.
- ✓The highly anisotropic 2D layered materials, such as BP and ReS_2, provide another attractive platform for FETs with gates smaller than 10 nm.

FURTHER RESEARCH OPPORTUNITIES

- ❑ Check the variation of magnetic moment by varying the stacking orders and to estimate the ground state configuration.
- ❑ Verify the relative stability of various stacking order with respect to the bulk state.

REFERENCES

1) G. Fiori, F. Bonaccorso, G. Iannaccone, T. Palacios, D. Neumaier, A. Seabaugh, S. K. Banerjee and L. Colombo, Nat. Nanotechnol., 2014, 9, 768–779.
2) 2.Wen Zhang, Lei Zhang, Ping Kwan Johnny Wong, Jiaren Yuan, Giovanni Vinai, Piero Torelli, Gerrit van der Laan, Yuan Ping Feng, and Andrew T. S. Wee. ACS Nano. 2019, 13(8), 8997-9004.
3) Bayard, M.; Sienko, M. J. J. Solid State Chem. 1976, 19, 325−329