Electronic Properties of Group IV Mono-Chalcogenides 2D Materials - Magnetism in 2D Materials

Student: Mehrshad Mehboudi Degree: Ph.D., May 2018
Major Professor: Dr. Salvador Barraza-Lopez

UNIVERSITY OF ARKANSAS
Graduate School & International Education
Microelectronics-Photonics

Modeling & Simulation

Background/Relevance

- Two dimensional atomic materials –consisting of only one sheet of atoms- are studied extensively since 2005.
- Group IV mono-chalcogenides are layered materials that can in principle be exfoliated down to a single layer.
- Monolayer of $CrSiTe_3$ is a 2D material with magnetism behavior.

Innovation

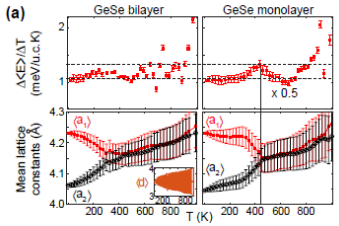
- Realization of structural phase transitions that modify material properties of 2D materials.
- Realization of asymmetric atomic structure in $CrSiTe_3$.

Approach

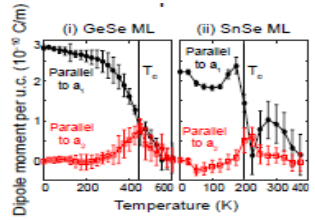
- Car-Parrinello Molecular Dynamics with SIESTA DFT code; analysis of instantaneous average structures to extract changes in material properties.
- Density functional theory as implemented in VASP code will be used to investigate electronic band structure, ionic and electronic polarization.
- SIESTA code will be use to calculate optical properties of monolayer of monochalcogenides.
- For $CrSiTe_3$, the total energy of the structure at symmetric and asymmetric conditions were calculated and compared.

Key Results

- Monochalcogenide monolayers undergo structural disorder before melting point. This disorder is in the form of bond reassignment
- Dipole moment of unit cell which contributes to piezoelectric effect reduces vs temperature as a result of disorder.



The average constants will be equal at the transition temperature.



Evolution of Dipole moment by temperature.

Conclusions

- There are strong effect of phase transition on the properties of monolayer of monochalcogenides.
- $CrSiTe_3$ monolayer is anti-ferromagnetic and has an asymmetric structure

Future Work

- Phonon calculation of symmetric and asymmetric structure gives better understanding of the ground state of CrSiTe3 monolayer.

References and Acknowledgement.

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- M. Mehboudi, B.M. Fregoso, Y. Yang, W. Zhu, A. van der Zande, J. Ferrer, L. Bellaiche, P. Kumar, and S. Barraza-Lopez, , 2016. Structural phase transition and material properties of few-layer monochalcogenides. arXiv preprint arXiv:1603.03748.
- Calculations have been performed on Arkansas Razor and Trestles HPC.
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