Effect of Mn-Doping and Strain on Magnetic and Electronic Properties of $MoSe_2$

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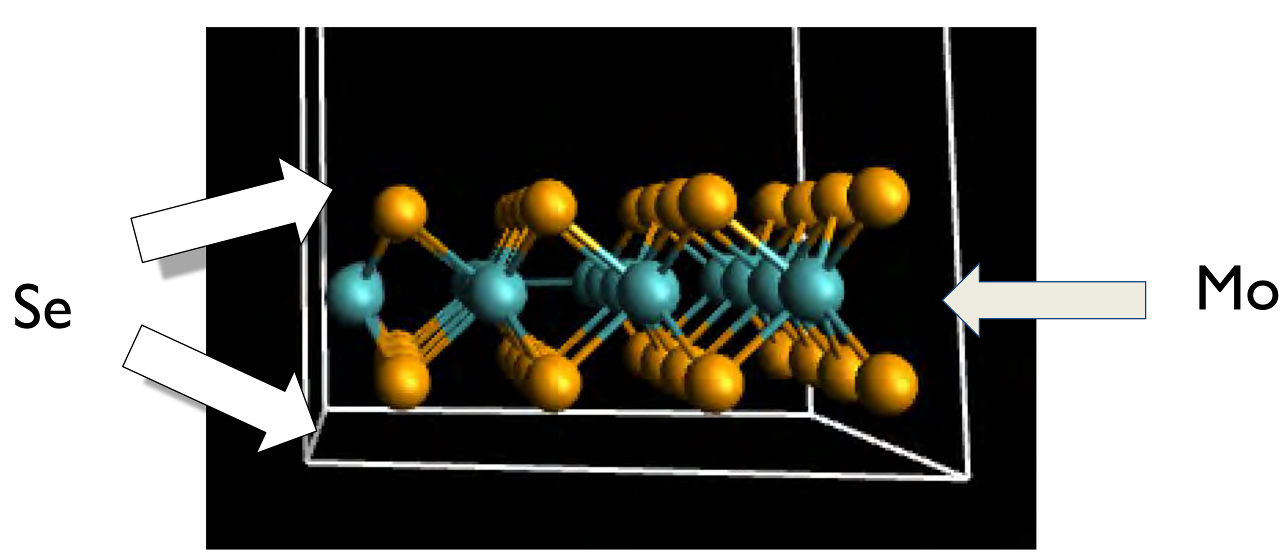
Summary

Transition metal dichalcogenides (TMDs) have recently become the focus of increased attention for their use as two-dimensional materials in digital electronic and spintronic applications. Their properties can potentially be modified and optimized for specific applications via doping or applying strain. The purpose of this study is to observe the effects of substitutional Mn-doping and strain on the magnetic, optical, and electronic properties of a monolayer of $MoSe_2$.

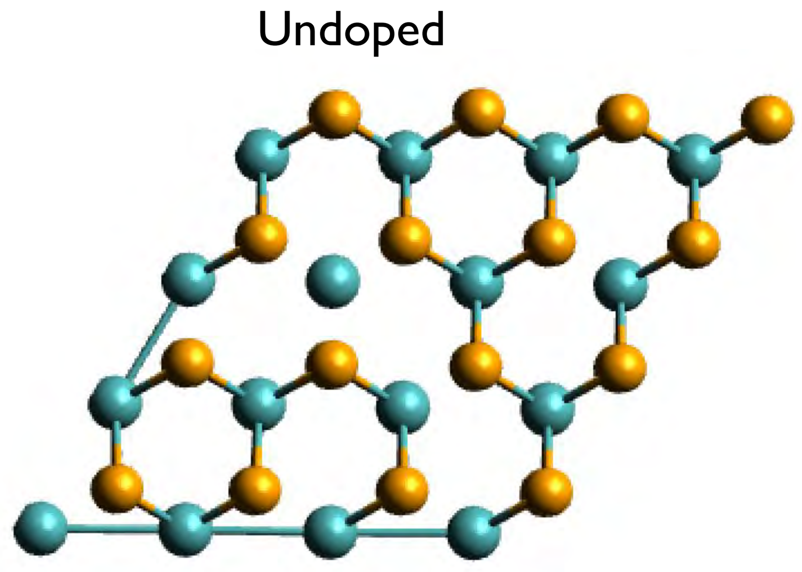
Introduction

Transition Metal Dichalcogenides (TMDs):
- 2D semiconductors
- Electronic and magnetic properties can be modified by doping or strain
- Molybdenum diselenide ($MoSe_2$) was researched in the study



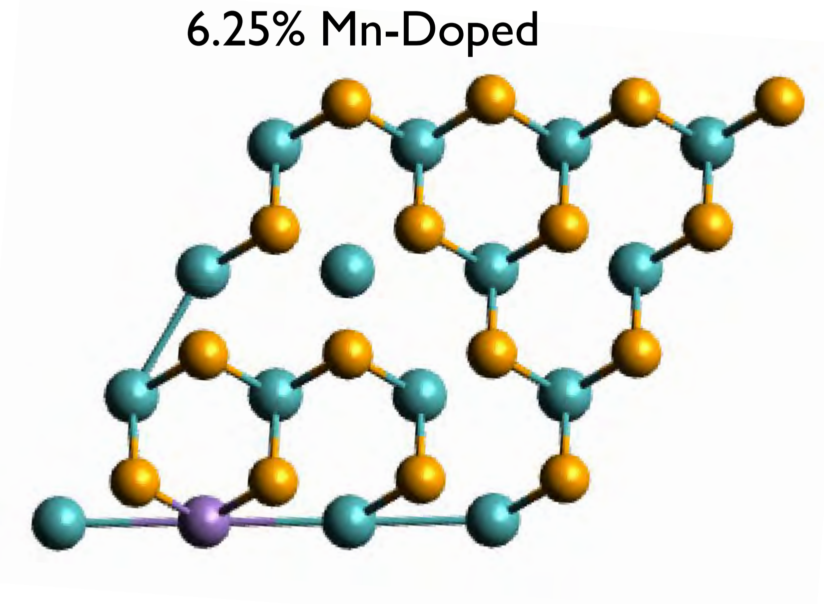
Calculation Methods

Undoped

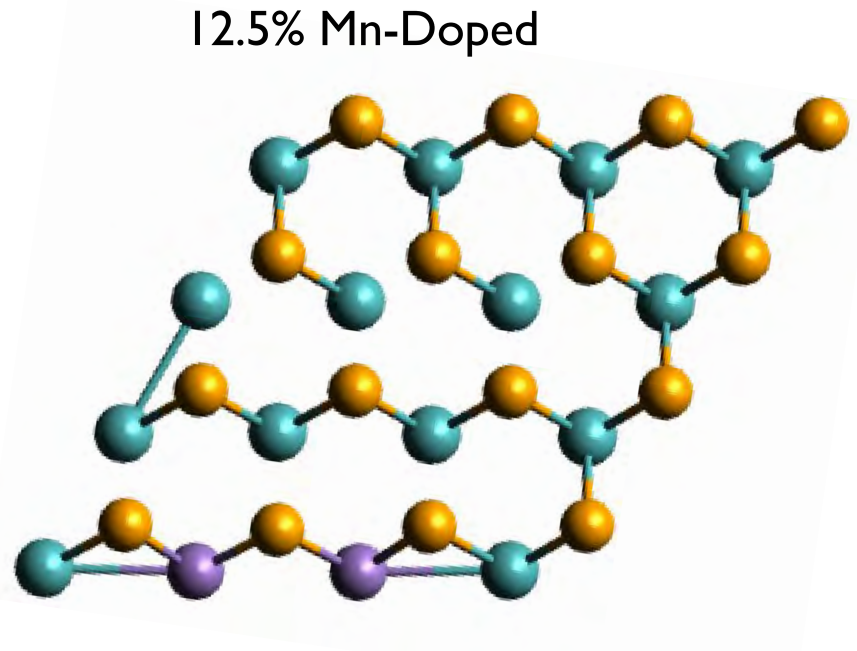


Key:
Orange = Selenium
Blue = Molybdenum
Purple = Manganese

6.25% Mn-Doped

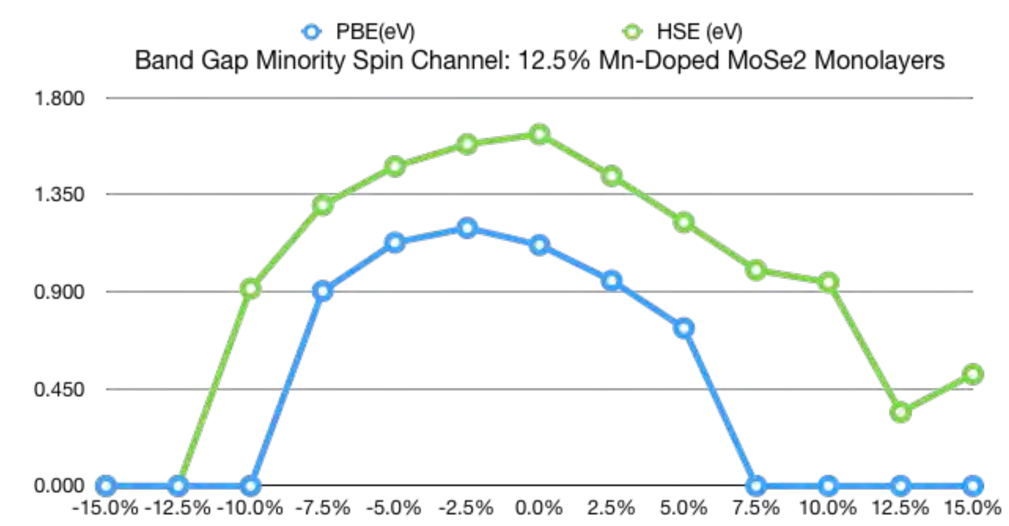


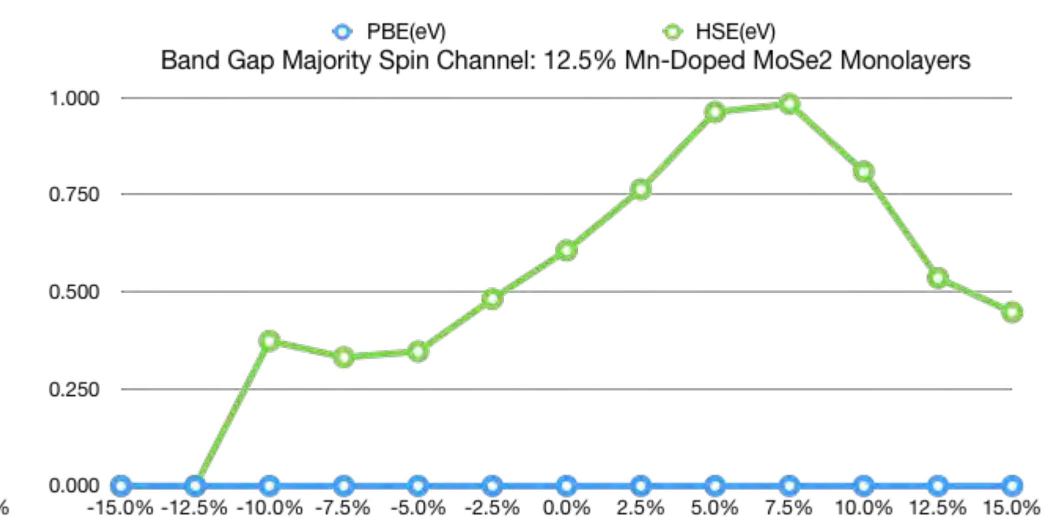
12.5% Mn-Doped



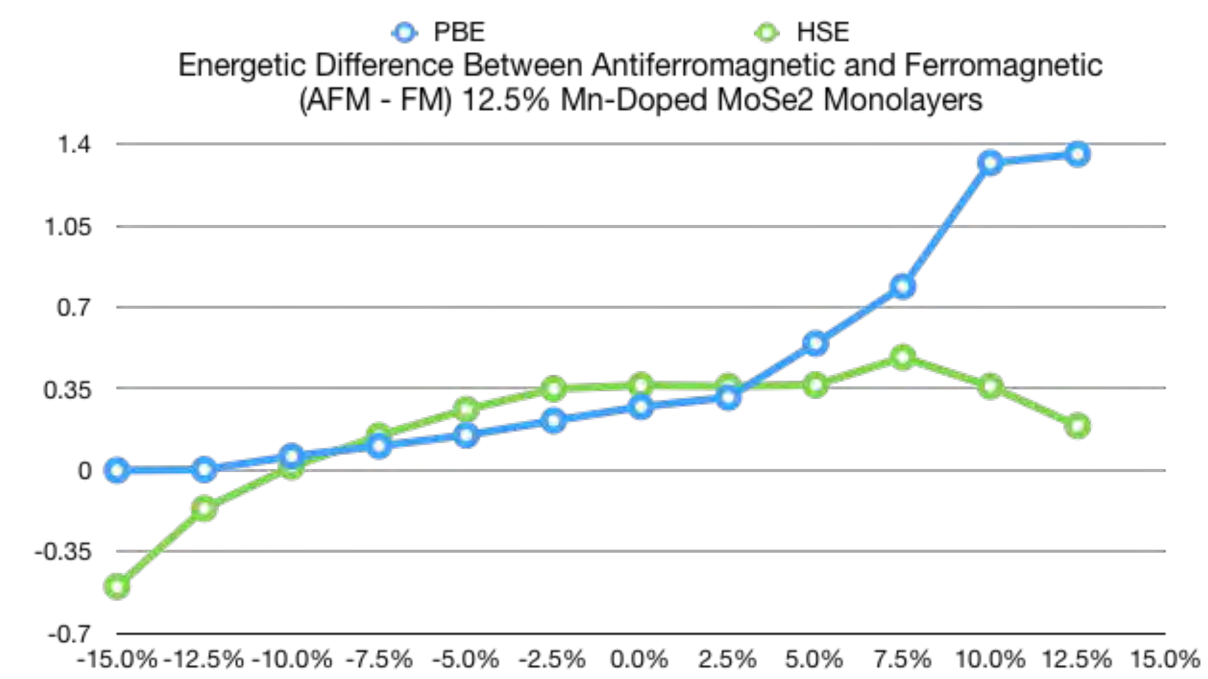
- Investigated pure $MoSe_2$ as well as doped with Mn at 6.25% and 12.5% concentrations
- Strain applied from -15.0% to 15.0% at 2.5% increments between data points
- Calculations run using density functional theory (DFT)
- PBE and HSE functionals

Results/Discussion

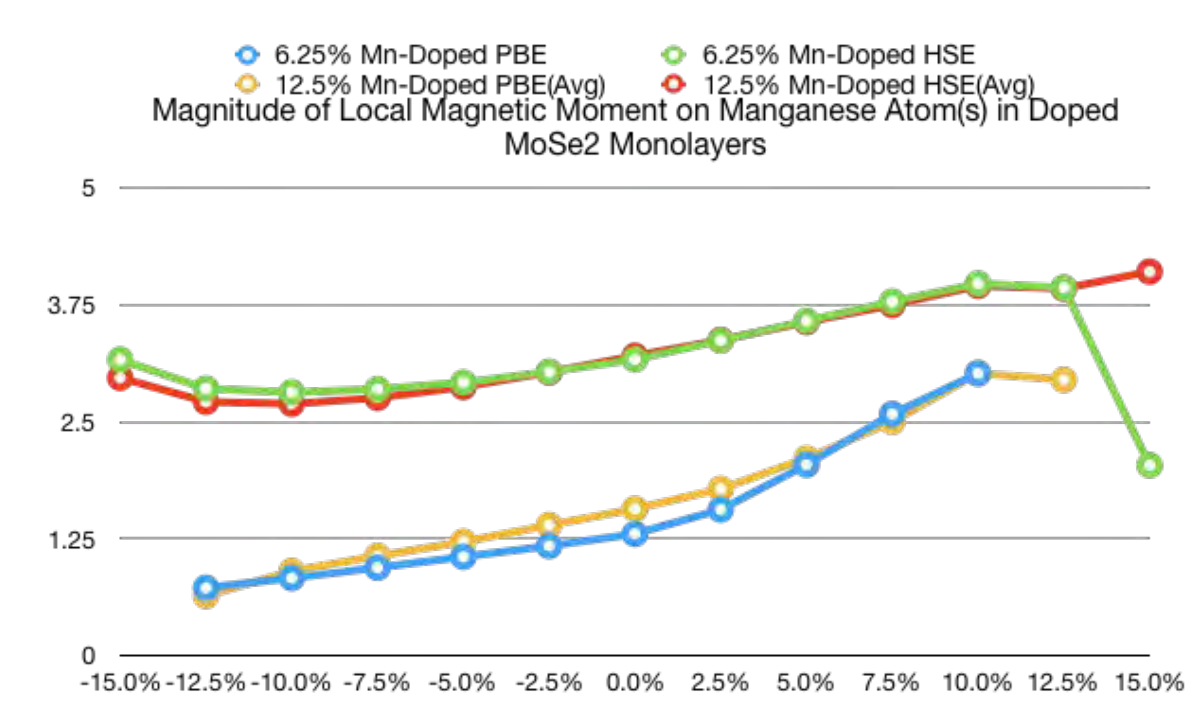




- Band gap decreases with increasing percentages of tensile and compressive strain
- PBE: half-metal structures -> metallic structures
- HSE: semiconductors -> metallic structures



Driving force for ferromagnetic ordering increased with increasing tensile strain and decreasing compressive strain



Local magnetic moments on Mn dopants increased with increasing tensile strain and decreasing compressive strain

Conclusions and Future Work

- Doping with Mn and applying strain can modulate semiconducting/metallic character
- Applying tensile strain can promote ferromagnetic ordering in Mn-doped $MoSe_2$
- Will refine trends with smaller intervals of strain percentages
- Will further study the shift from direct to indirect band gaps

Acknowledgments

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