Effect of Mn-Doping and Strain on Magnetic and Electronic Properties of MoSe$_2$

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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$_2$.

**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$_2$.

**Results/Discussion**

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

**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**

- 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

**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

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