Magnetic Spinel Chalcogenides: A Possible New Class of Spintronic Material

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Abstract

The goal of the project is to synthesize and study the properties of magnetic spinel chalcogenides:
- CuCr₂Se₄ has a Curie temperature ($T_c$) higher than room temperature and is metallic.
- CdCr₂Se₄ is a magnetic semiconductor with interesting magneto-optical and electronic properties.
- Semiconductor nanocrystals exhibit quantum confinement effects such as size-dependent optical and electronic properties that are useful for applications.
- We expect the chalcospinel solid solution CdₓCu₁₋ₓCr₂Se₄ to exhibit tunable magnetic and semiconducting properties.

Experimental

Cu-oleate complex, Cr-oleate complex in oleylamine

Inject

Se powder with β-sitosterol in Tri-octylamine heated to 350°C

The reaction is maintained at 350°C for 3 hours

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(a) Magnetization as a function of magnetic field for CuCr₂Se₄ nanocrystals measured using AGM.
(b) TEM image of CuCr₂Se₄ nanocrystals.

Crystal structure of the chalcospinel showing the octahedral and tetrahedral site position of Cr and Cu ions in the lattice.

The following cell was built for theoretical calculation by using Vienna ab-initio simulation package (VASP) based on density functional theory (DFT).

The XRD pattern for CuCr₂Se₄ nanocrystals.

- The density of states (DOS) of the CuCr₂Se₄ majority and minority bands. The solid line is the total DOS and the dotted line is the DOS of the chromium $d$-orbital.
- This is a metallic ferromagnet with a magnetic moment 5.09μB per formula unit.

DOS for CdₓCu₁₋ₓCr₂Se₄

- This is predicted to be half-metallic with a magnetic moment 5.50μB per formula unit.

DOS for CdCr₂Se₄

- This is a semiconducting ferromagnet with a magnetic moment 6.00μB per formula unit.

Conclusion

- Well dispersed nanocrystals of CuCr₂Se₄ have been synthesized using solution chemistry.
- Theoretical calculation show that CuCr₂Se₄ is a metallic ferromagnet and CdCr₂Se₄ is a semiconducting ferromagnet consistent with experimental observation. CdₓCu₁₋ₓCr₂Se₄ is predicted to be half-metallic.

Future Work

- Expand to synthesis of CdCr₂Se₄ and CdₓCu₁₋ₓCr₂Se₄ nanocrystals and explore properties. Explore growth of thin films of the chalcospinels using chemical vapor deposition (CVD).
- Band structure calculations of Cd-Cu chalcospinel alloy compositions.