Investigation of Optical Properties of PbSe/PbX Core/Shell Nanocrystals

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Background/Relevance

- PbSe is a useful material for detection in the infrared, but oxidation reduces the functionality of the material in device applications.

Innovation

- Utilize WIEN2k, a program that performs electronic structure calculations, to model PbSe, and PbSe/PbS core/shell nanocrystals.

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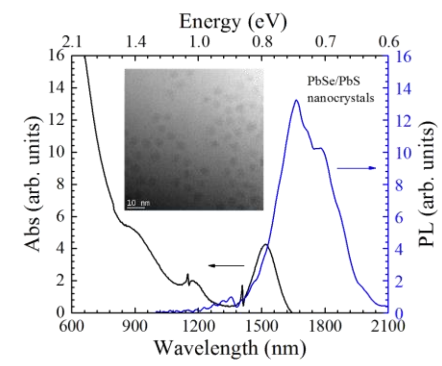
Approach

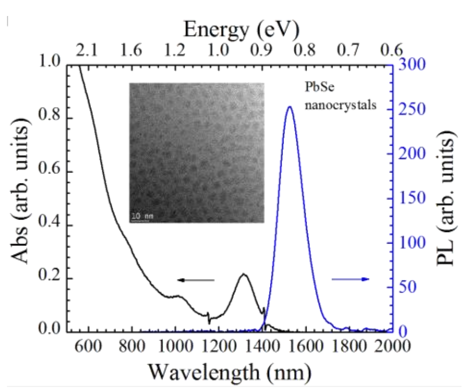
- Model PbSe nanocrystals with different shells and of various sizes using WIEN2k.
- Synthesize the material using a wet chemical method.
- Optimize the shell growth procedures.
- Characterize the nanocrystal structures through TEM imaging, absorbance, and photoluminescence measurements.



Absorbance and photoluminescence of PbSe/PbS nanocrystals grown at 120°C for 15 min.

Key Results

- Modeling PbSe in WIEN2k.
- Successful wet chemical synthesis of PbSe nanocrystals.
- Successful PbSe/PbS core/shell synthesis procedure.
- Absorbance and photoluminescence measurements



Absorbance and photoluminescence of PbSe nanocrystals grown at 140°C for 20s.

Conclusions

- Oxidation of PbSe nanocrystals incorporated into a photodetector degrades the performance of the device, and necessitates a shielding of some sort.
- The PbS shell provides protection for the PbSe core. The addition of the shell also red shifts the absorbance and emission spectra.

Future Work

- Another possible variation is an alloyed shell where the shell is composed of a ratio of lead sulfide and lead selenide, $PbSe/PbSe_xPbS_{1-x}$.