

Reduced Electron-Phonon Coupling and Enhanced Charge Transfer in Solar Cell Nanomaterials

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Sponsor: NSF

QUANTITATIVE IMPACT

OBJECTIVES

Synthesize high-crystallinity monodisperse semiconductor nanocrystals of various shapes

- High crystallinity is essential in enhancing charge transportation in nanocrystals.
- Identification of shape influence on the NC properties is essential in choosing best materials for solar applications.

Study phonon-assisted hot electron relaxation dynamics

- Understanding energy relaxation mechanisms is essential in reducing energy loss and improving energy conversion efficiency in solar cell devices.

METHODS

Synthesis

- Pyrolysis of organo-metallic compounds was used.
- Modifications were made in parameters, like surfactant, solvent, precursor, temperature.

Simulation

- Time-domain non-adiabatic molecular dynamics simulation was realized by implementing the fewest switching surface hopping (FSSH) technique in the time-domain Kohn-Sham (TDKS) theory.

KEY RESULTS AND FINDINGS:

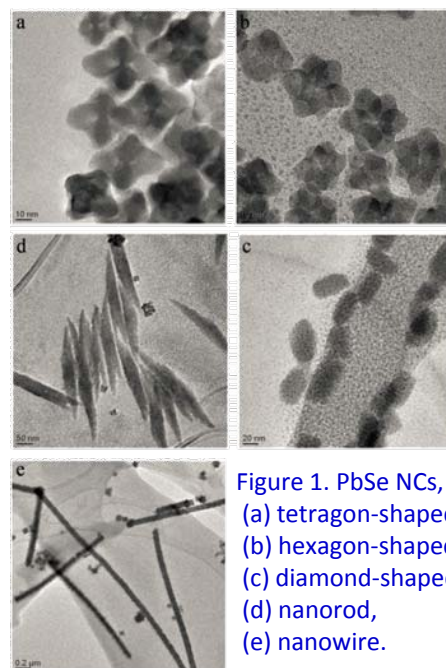


Figure 1. PbSe NCs, (a) tetragon-shaped, (b) hexagon-shaped, (c) diamond-shaped, (d) nanorod, (e) nanowire.

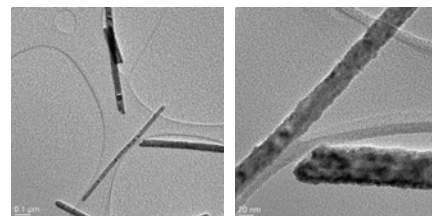


Figure 2. CdTe NWs.

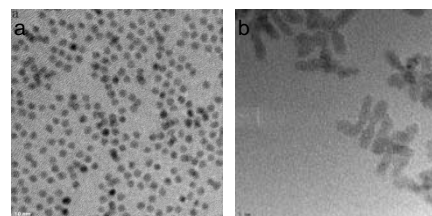


Figure 3. CdSe NCs. (a) spherical, (b) nanowire.

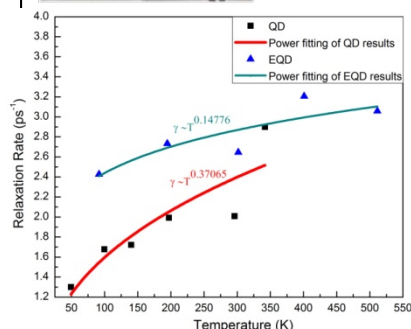


Figure 4. Hot electron relaxation rate as a function of temperature for the CdSe QD and EQD.

The relaxation of hot electrons proceeds faster and shows stronger temperature dependence in the EQD than in the QD.

Impact

- Various shapes of semiconductor NCs were produced using this simple one-step synthesis method.
- Influence of shape and temperature on the hot electron relaxation dynamics were understood.

Applications

- Rational selection of materials for semiconductor NC-based solar cell device.
- More experimental inputs for the study of shape influences on the NC properties.

Selected Publications

- H. Bao, B.F. Habenicht, O.V. Prezhdo, and X.L. Ruan, *Phys. Rev. B* **79**, 235306-1-7, 2009.
- L. Chen, H. Bao, T. Tan, O. Prezhdo, and X. Ruan, *J. Phys. Chem. C* **115**, 11400, 2011.
- W.Z. Wu, Z.R. Zheng, and X.L. Ruan, *Nanotechnology* **21**, 265704, 2010.