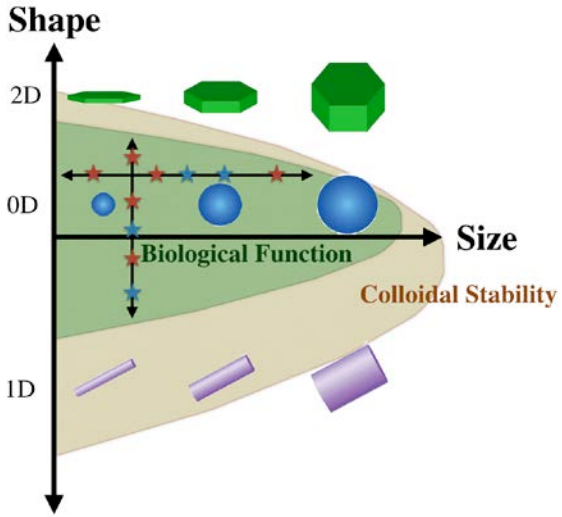
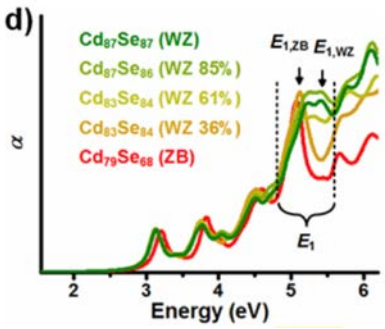
BLUE WATERS
SUSTAINED PETASCALE COMPUTING

Allocation: BW Professor/30 Knh; Illinois/550 Knh
PI: Andre Schleife
University of Illinois at Urbana-Champaign
Physics & Engineering

OPTICAL DETERMINATION OF CRYSTAL PHASE IN SEMICONDUCTOR NANOCRYSTALS





(Left) Shape and structure design space of semiconductor nanocrystals; (Right) Influence of crystal structure on optical properties.

Research Challenge

The fundamental connection between crystal structure and optical properties is not well understood, which hampers the use of nanocrystals in light-emitting diodes, solar cells, bioimaging, and consumer electronics. This research will establish a connection among the electronic and optical properties of semiconductor nanocrystals. This will allow tuning the size, shape, composition, and internal structure and accelerate the development of these materials.

Methods & Codes

Cadmium selenide is an inorganic compound with the formula CdSe. The team uses a combination of cutting-edge experimentation and theoretical spectroscopy to clarify important structure-property relationships for CdSe nanocrystals in two different crystal structures - wurtzite and zincblende. Simulations are accomplished with the Vienna Ab Initio Simulation Package (VASP: https://www.vasp.at) and solving the Bethe-Salpeter equation (https://en.wikipedia.org/wiki/Bethe–Salpeter_equation).

Results & Impact

CdSe-containing quantum-dot light-emitting diodes (QLEDs) are 5.4 times more efficient than previously reported similar devices.

It is possible to distinguish between the two crystal structures using optical absorption spectra and the Blue Waters calculations explain the band structure origin of the spectral features underlying this effect. The results pave the way for applying accelerated experimentation to nanocrystals in solution.

Why Blue Waters

The analyses are computationally extensive with large matrices that require well parallelized codes on fast supercomputers with fast inter-connects. These calculations are not possible on high throughput systems. The calculations utilize fast CPUs, large amounts of memory per compute core, and fast interconnects. Further, the Blue Waters SEAS staff helped identify and fix performance bottlenecks associated with writing and reading large wave function files.