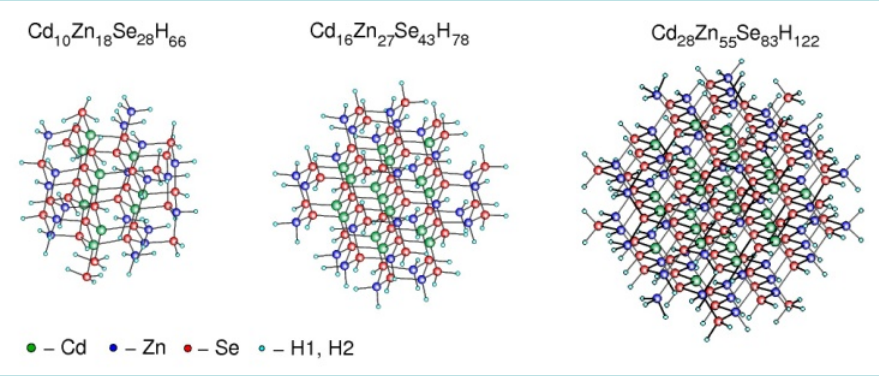
Core-Shell Heterostructures for Photovoltaic Energy Conversion

Igor Vasiliev, Department of Physics, New Mexico State University, Las Cruces, NM 88003

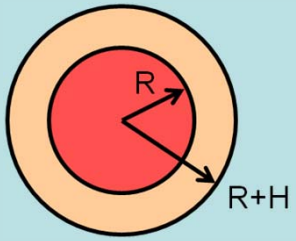
Our research focuses on theoretical prediction of the structural, electronic, and optical properties of core-shell semiconductor nanocrystals. The goal of this project is to expand the knowledge of chemistry and physics of semiconductor heterostructures and accelerate the development of composite materials for efficient conversion of solar energy.

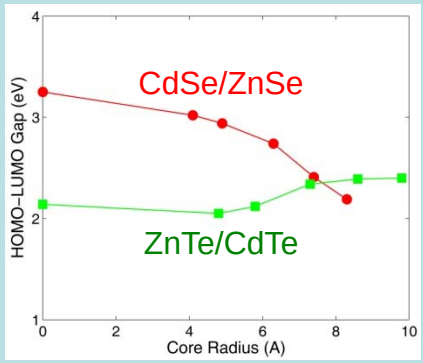
Ab initio density functional study of core-shell semiconductor nanocrystals

Two types of core-shell nanocrystals were studied: traditional, in which a core of a narrow gap semiconductor is covered with a shell of a wide gap material, and inverted, in which a wide-gap core is enclosed in a narrow-gap shell. Our calculations demonstrated that the HOMO-LUMO gaps in core-shell nanocrystals can be tuned by more than ~1 eV by adjusting the size of the core without changing the external diameter of the nanocrystals.



Structures of CdSe/ZnSe core-shell nanocrystals





CdSe core / ZnSe shell						
R (Å)	0	4.1	4.9	6.3	7.4	8.3
H (Å)	9.3	5.2	4.4	3.0	1.9	1.0
E_g (eV)	3.25	3.02	2.94	2.74	2.41	2.19
ZnTe core / CdTe shell						
R (Å)	0	4.8	5.8	7.3	8.6	9.8
H (Å)	11.0	6.2	5.2	3.7	2.4	1.2
E_g (eV)	2.14	2.05	2.12	2.34	2.39	2.40

Calculated HOMO-LUMO gaps in traditional CdSe/ZnSe and inverted ZnTe/CdTe nanocrystals