COE, Tohoku University,
February 2004

Semiconducting Nanoparticles:

Flexible Properties out of Tunable Sizes

Atoms+Molecules  **Condensed Matter**

The nanometric world

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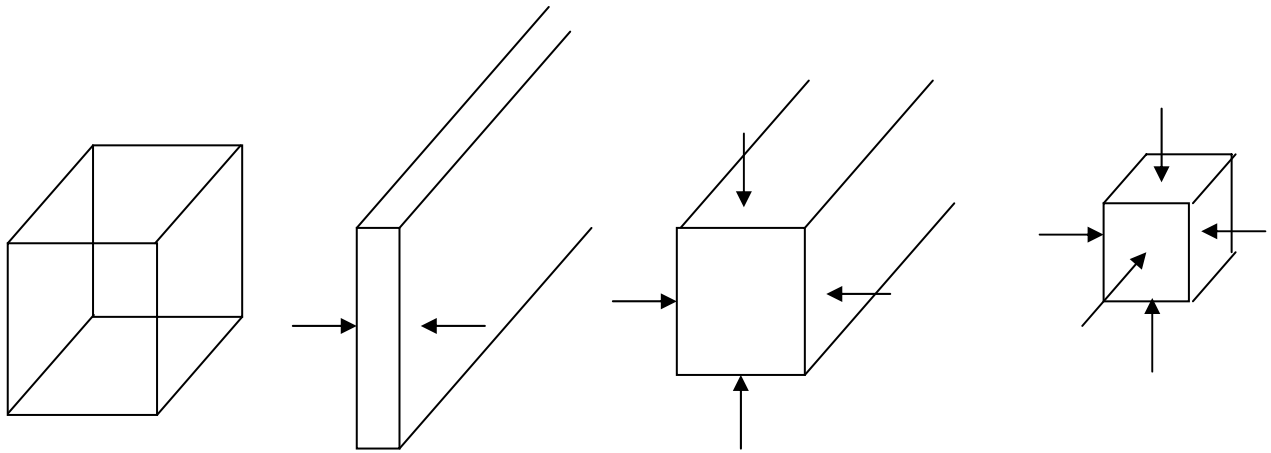
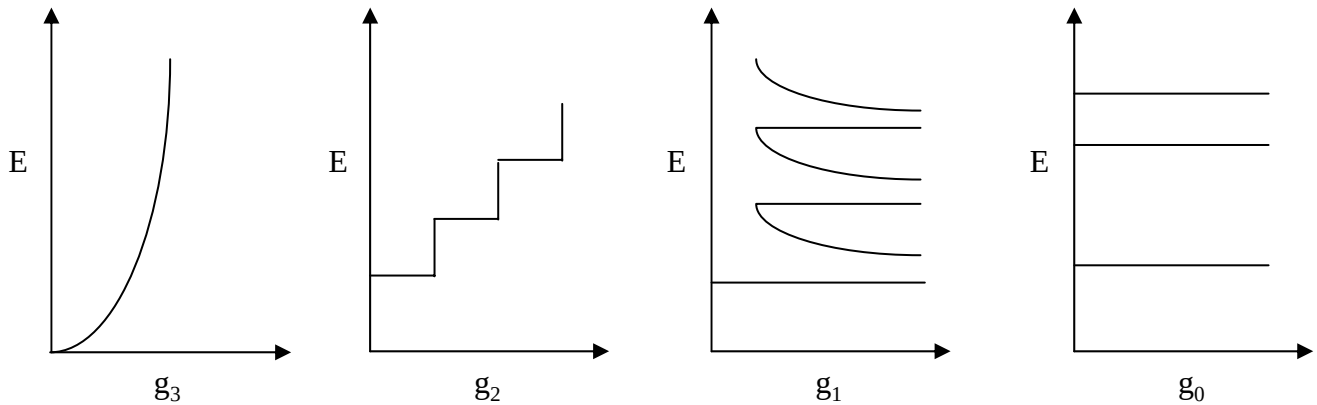


Bulk Thin Film Nanowire Quantum Dot



$E = \pi^2\hbar^2n^2/(8ma^2)$

Density of states (DOS)

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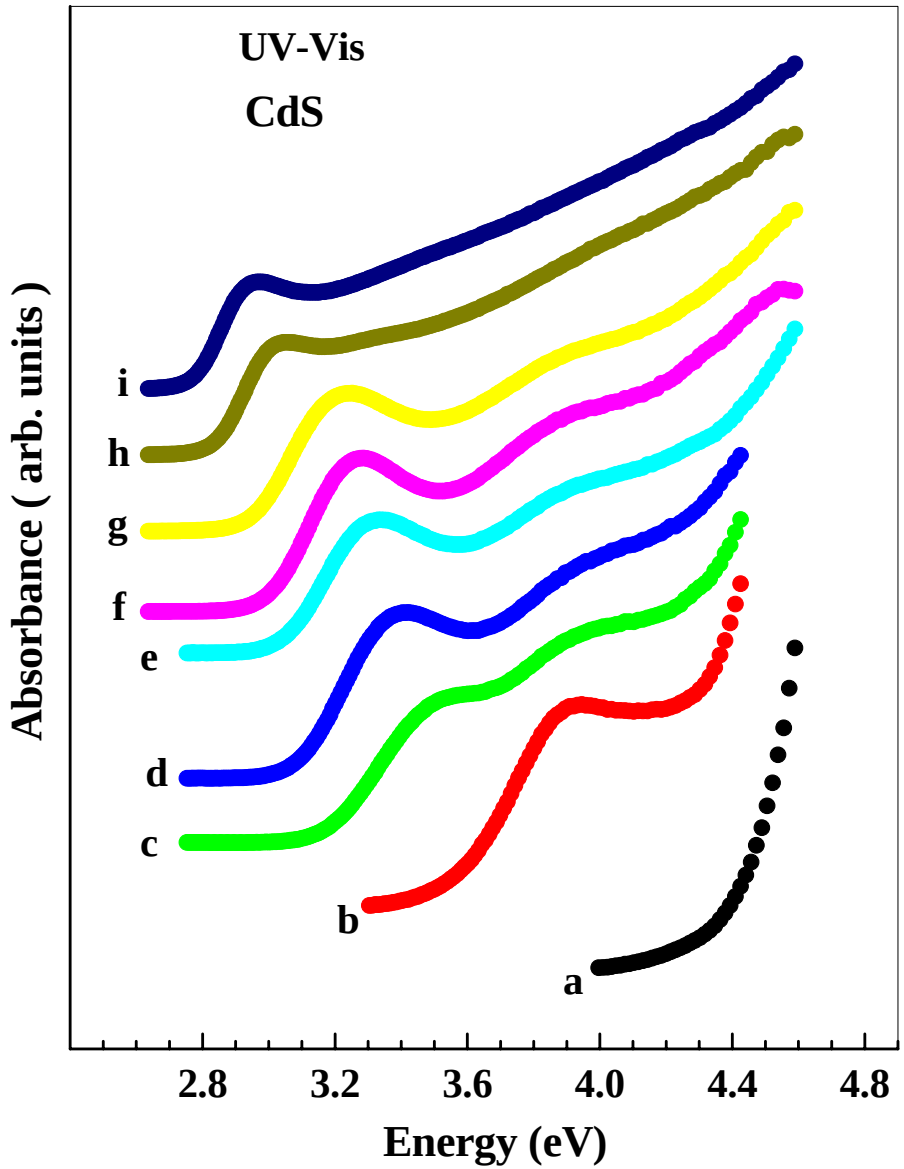
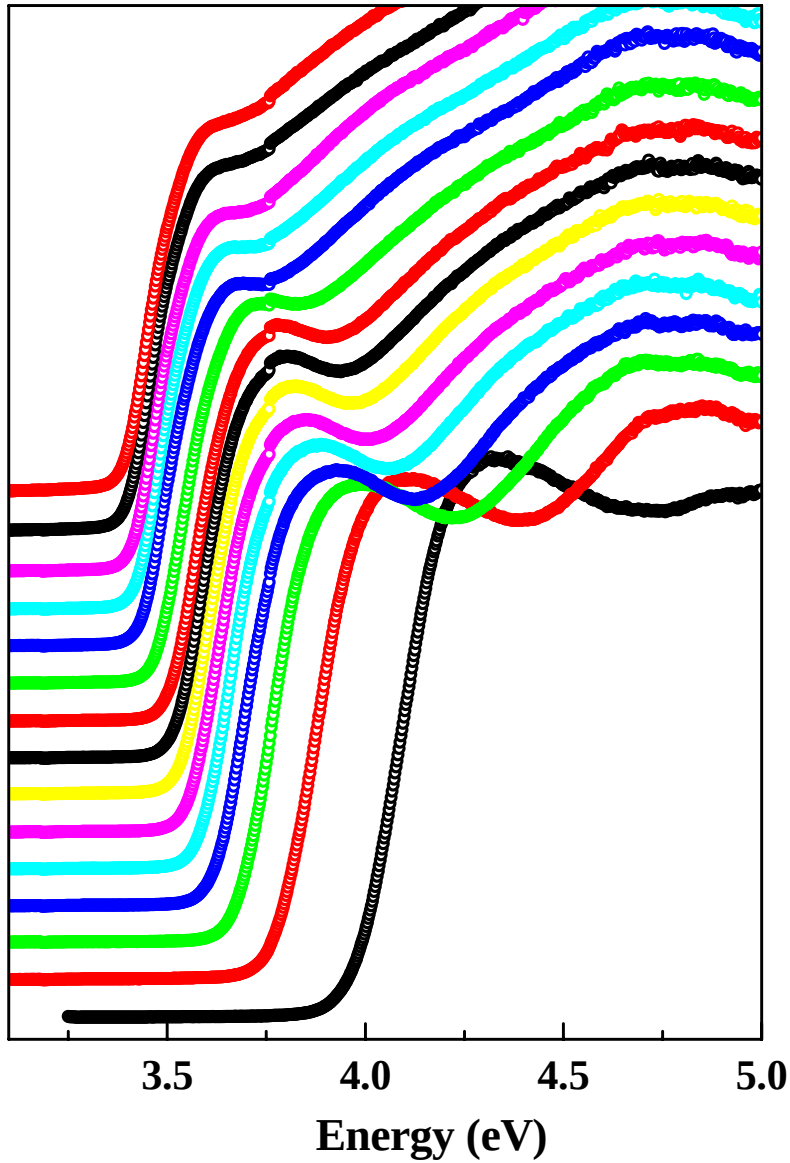
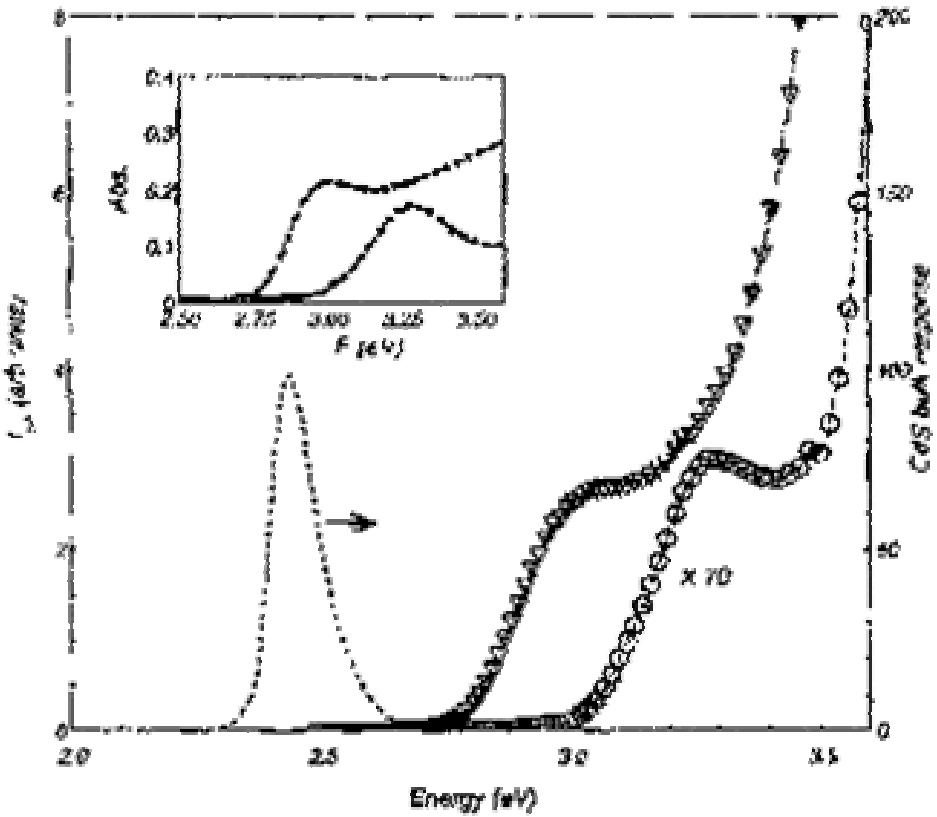
Band gap tuning of CdS and in ZnO

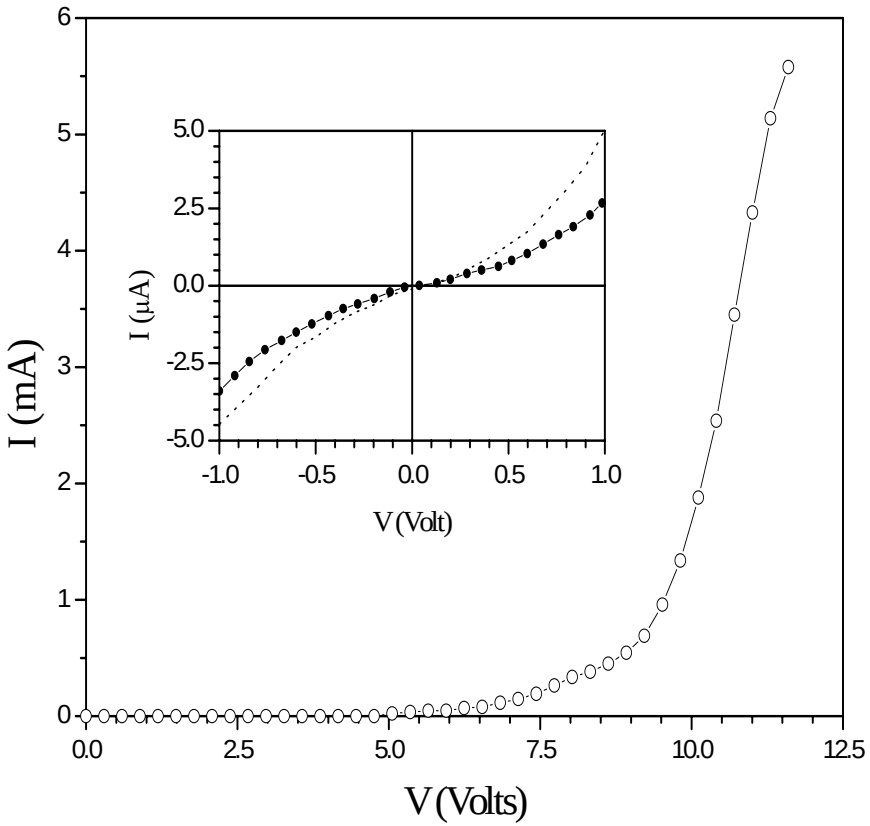




J. Nanda, Ph.D. Thesis, Bangalore; R. Viswanatha et al., to be published.

Photocurrent response from CdS





J. Nanda *et al.*, Appl. Phys. Lett. 72 (1998) 1335

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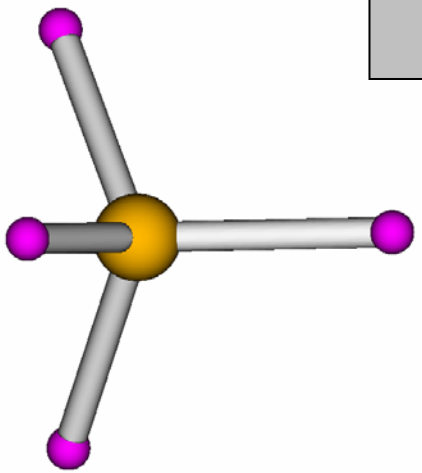
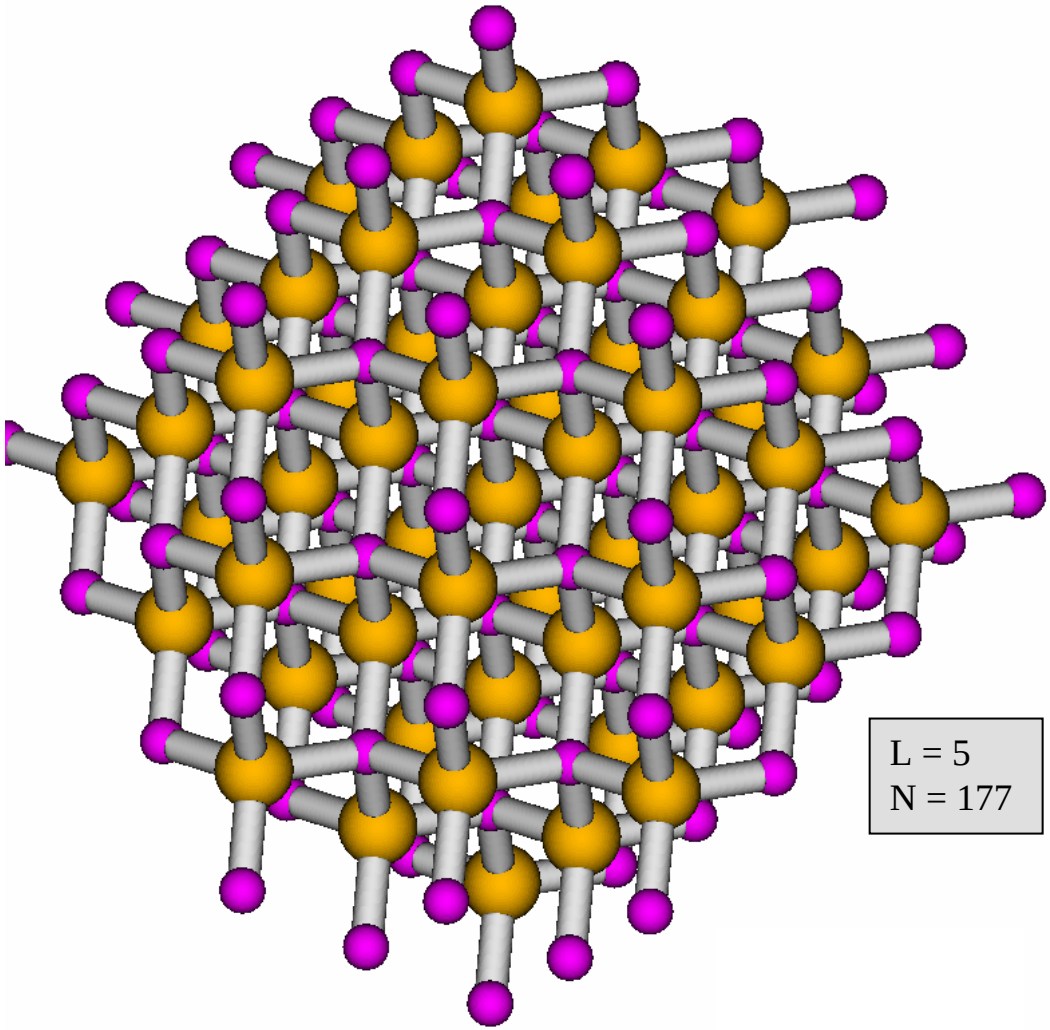
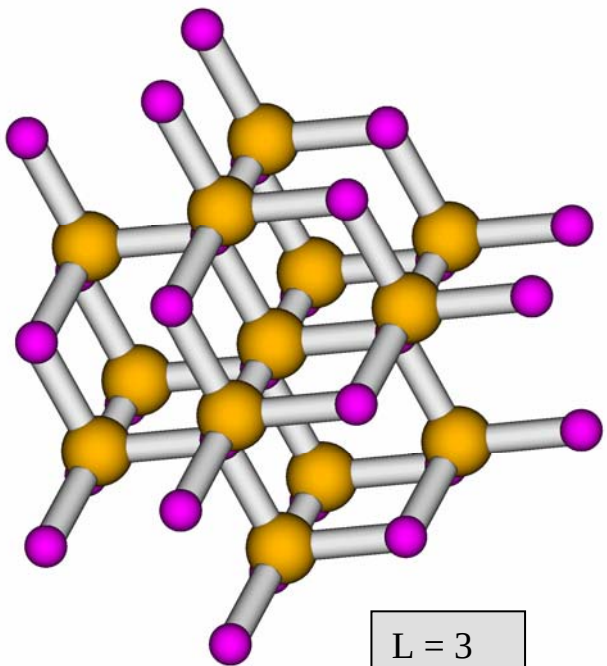
L – Number of layers
N – Number of atoms



L = 1
N = 5

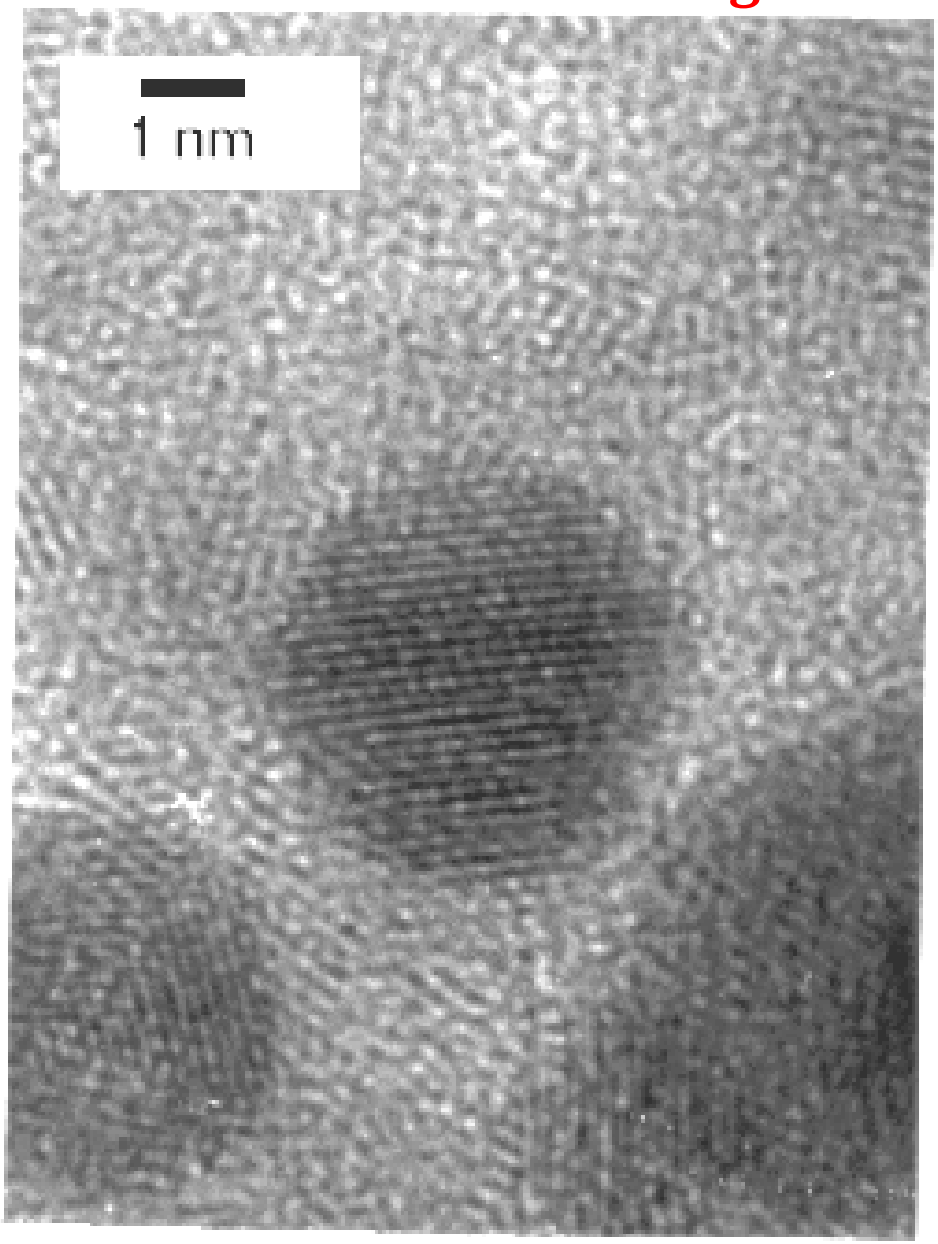


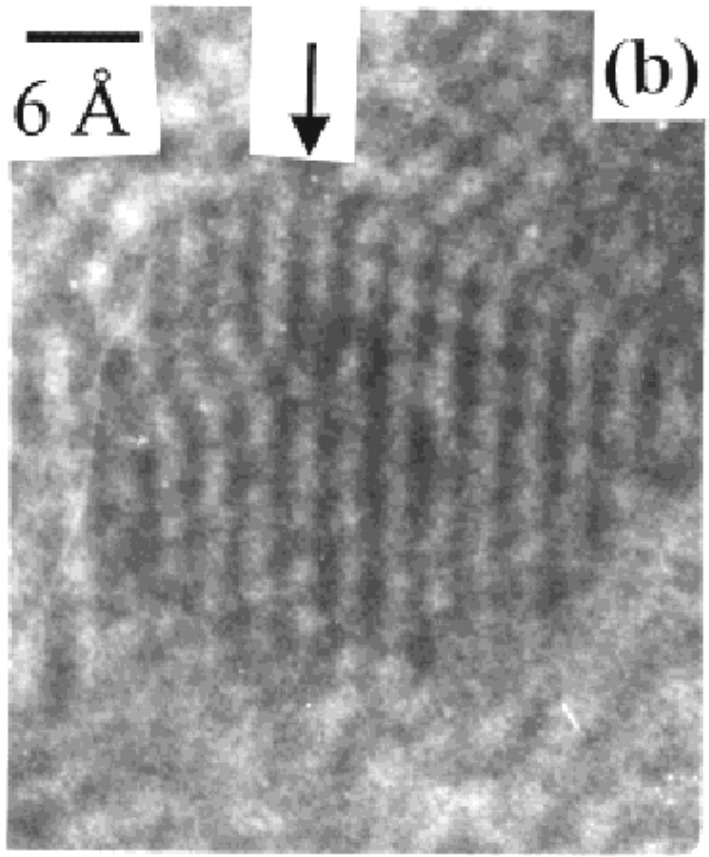
L = 5
N = 177



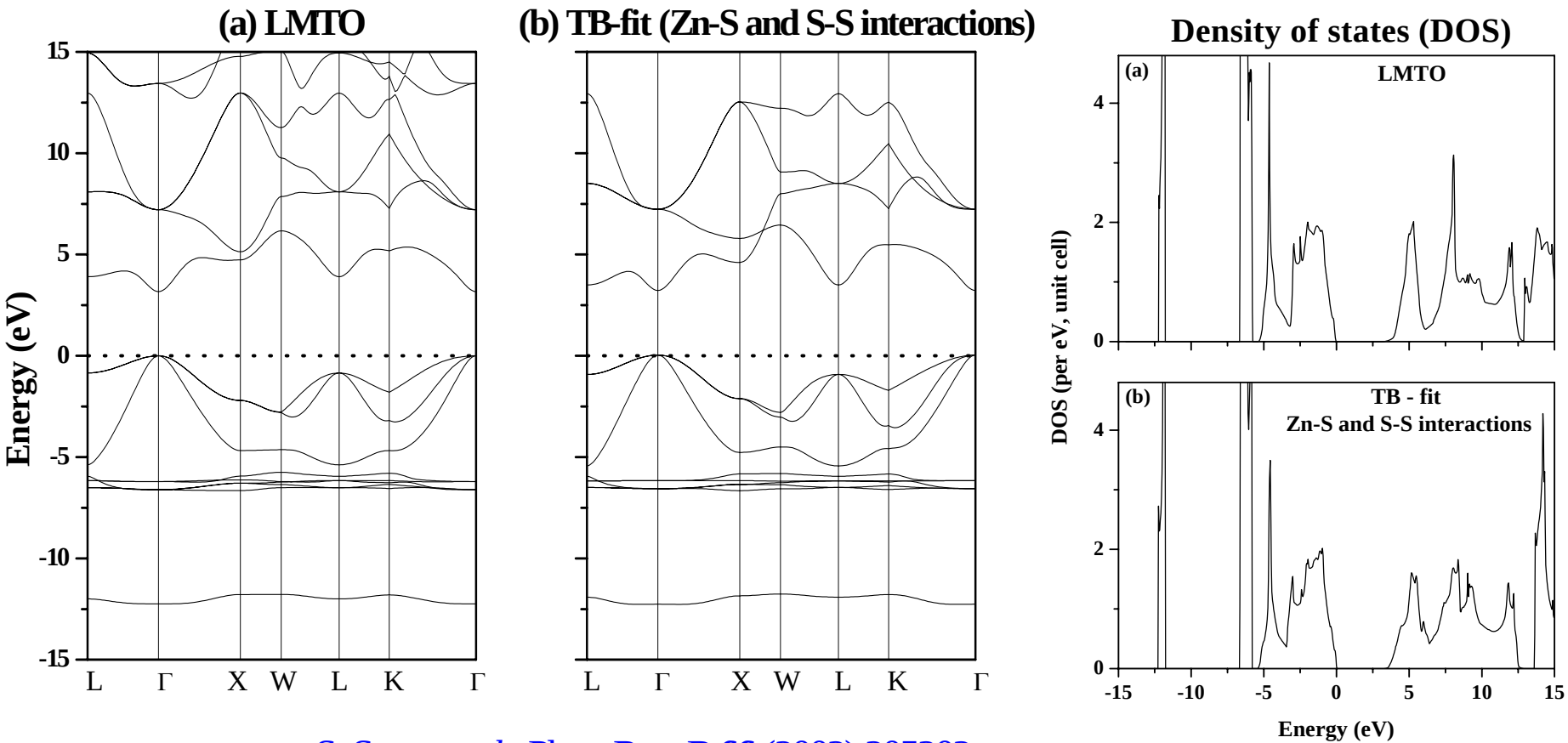
L = 3
N = 41

Seeing is believing





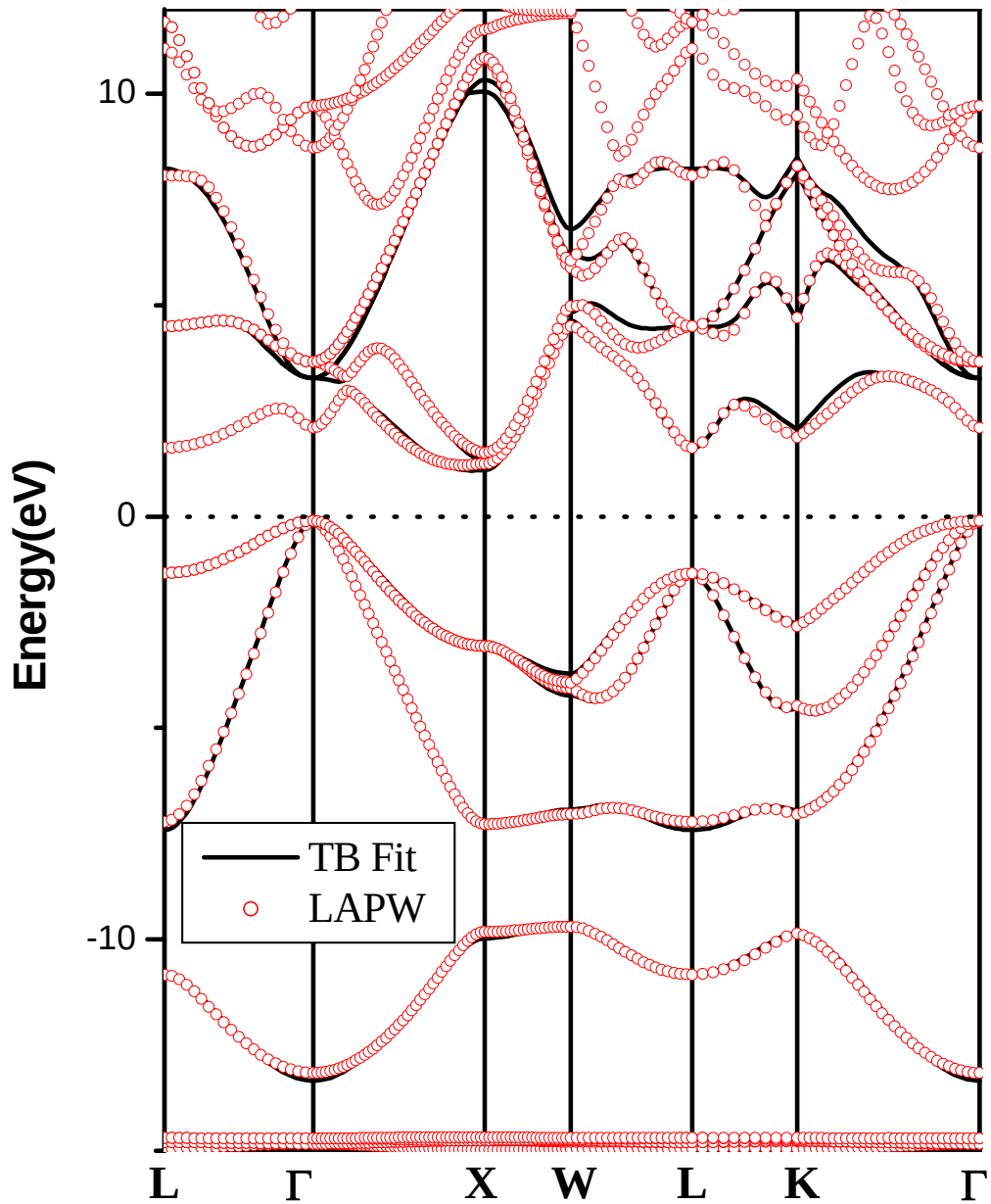
How do we describe the electronic structure?



S. Sapra *et al.*, Phys. Rev. B **66** (2002) 205202

COE, Tohoku University,
February 2004

BAND STRUCTURE OF GaP



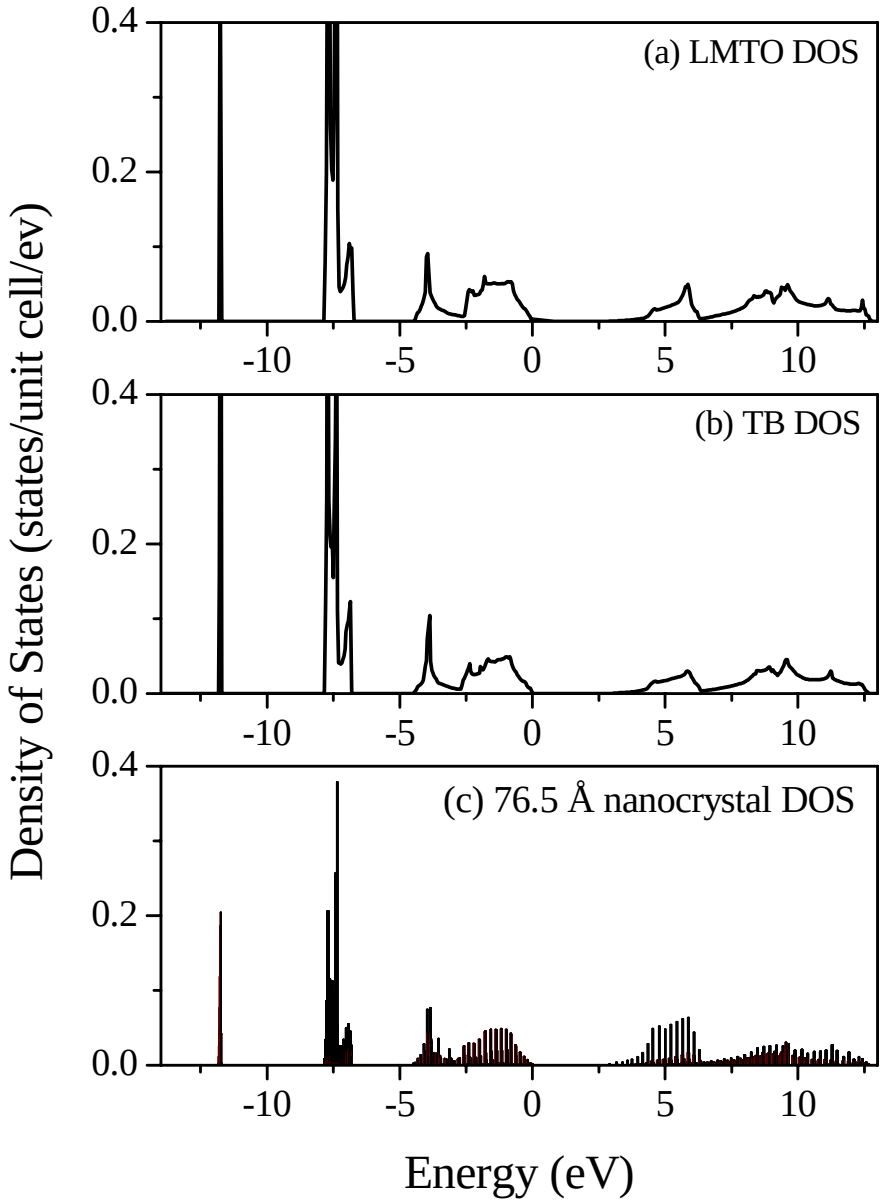


Fig. 1, Sapra and Sarma

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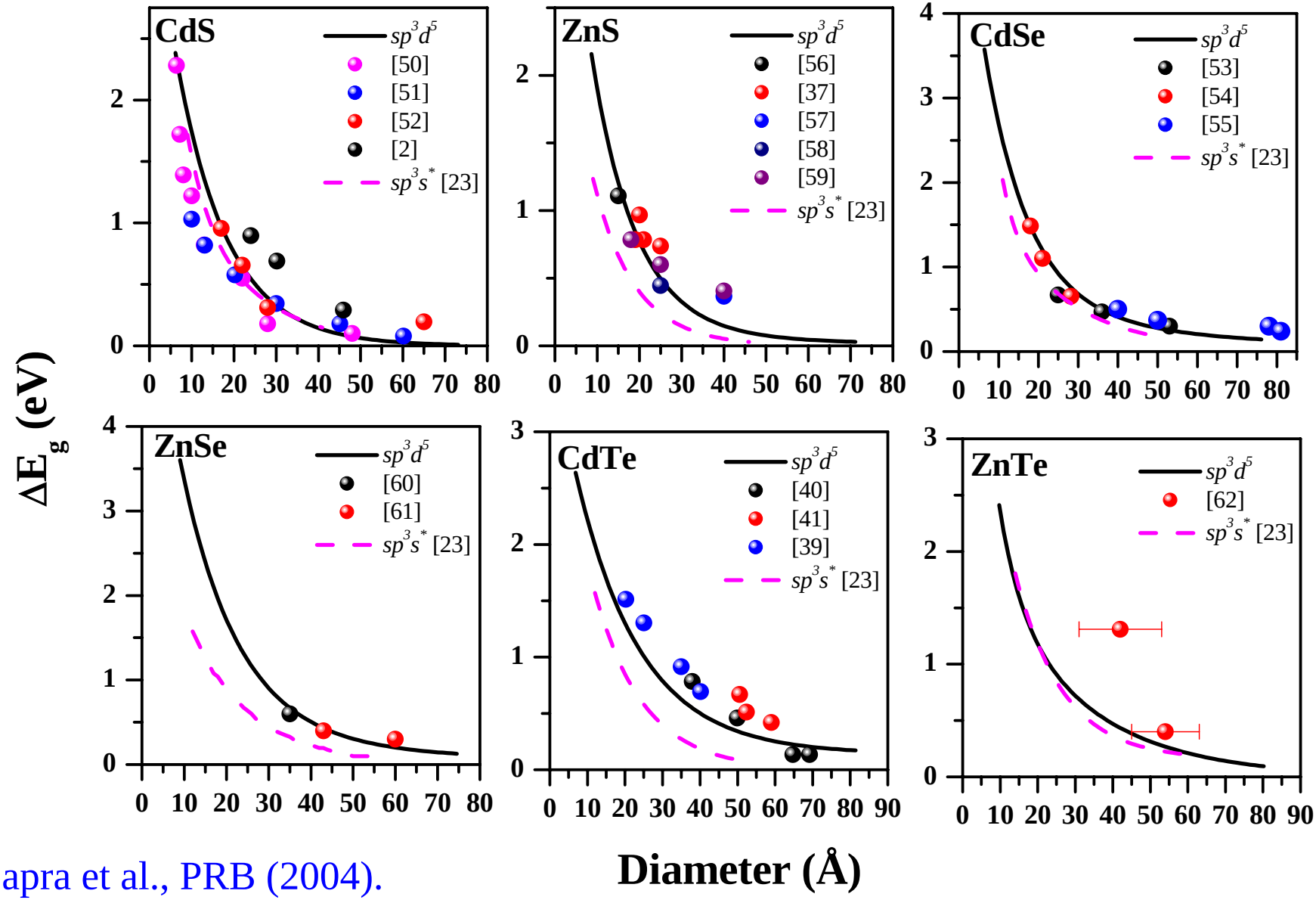
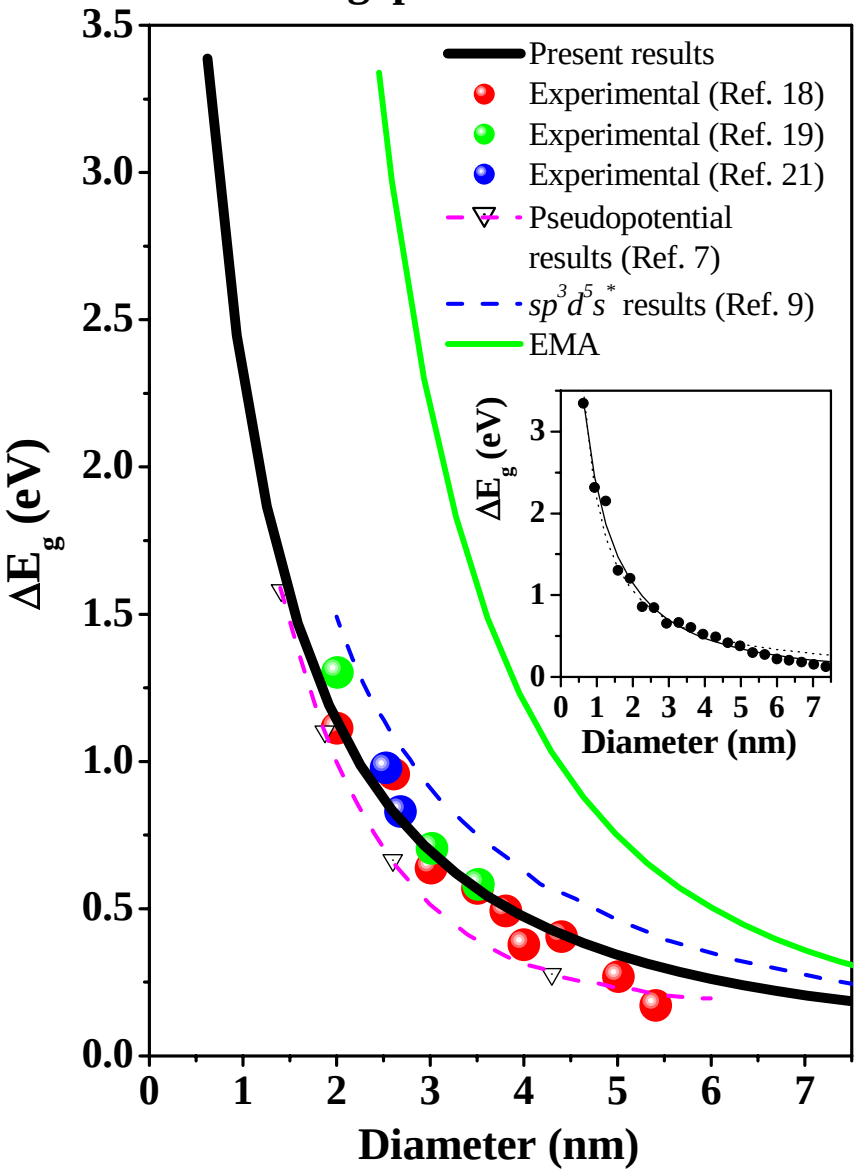
Bandgap variation in II-VI semiconductors with size



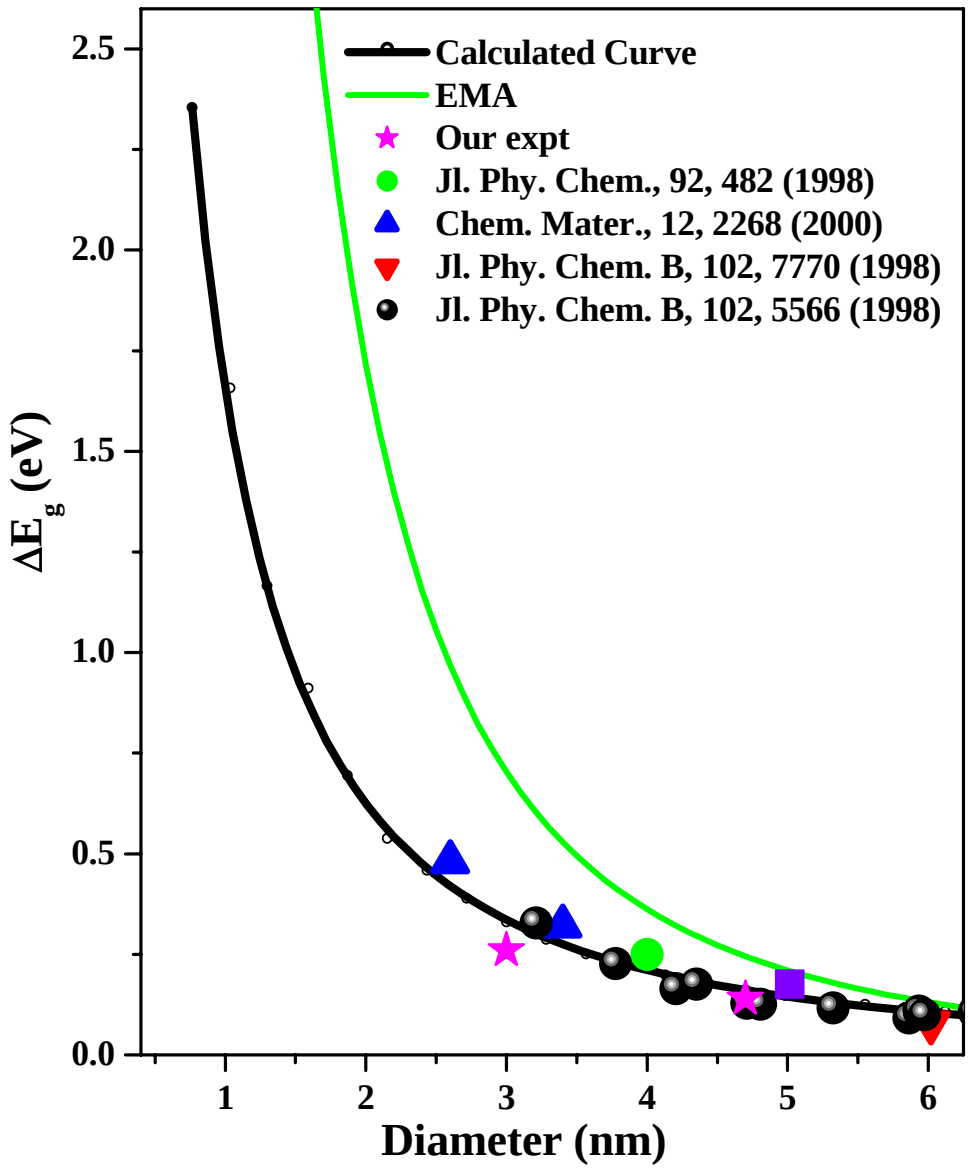
Sapra et al., PRB (2004).

Bandgap variation in InP



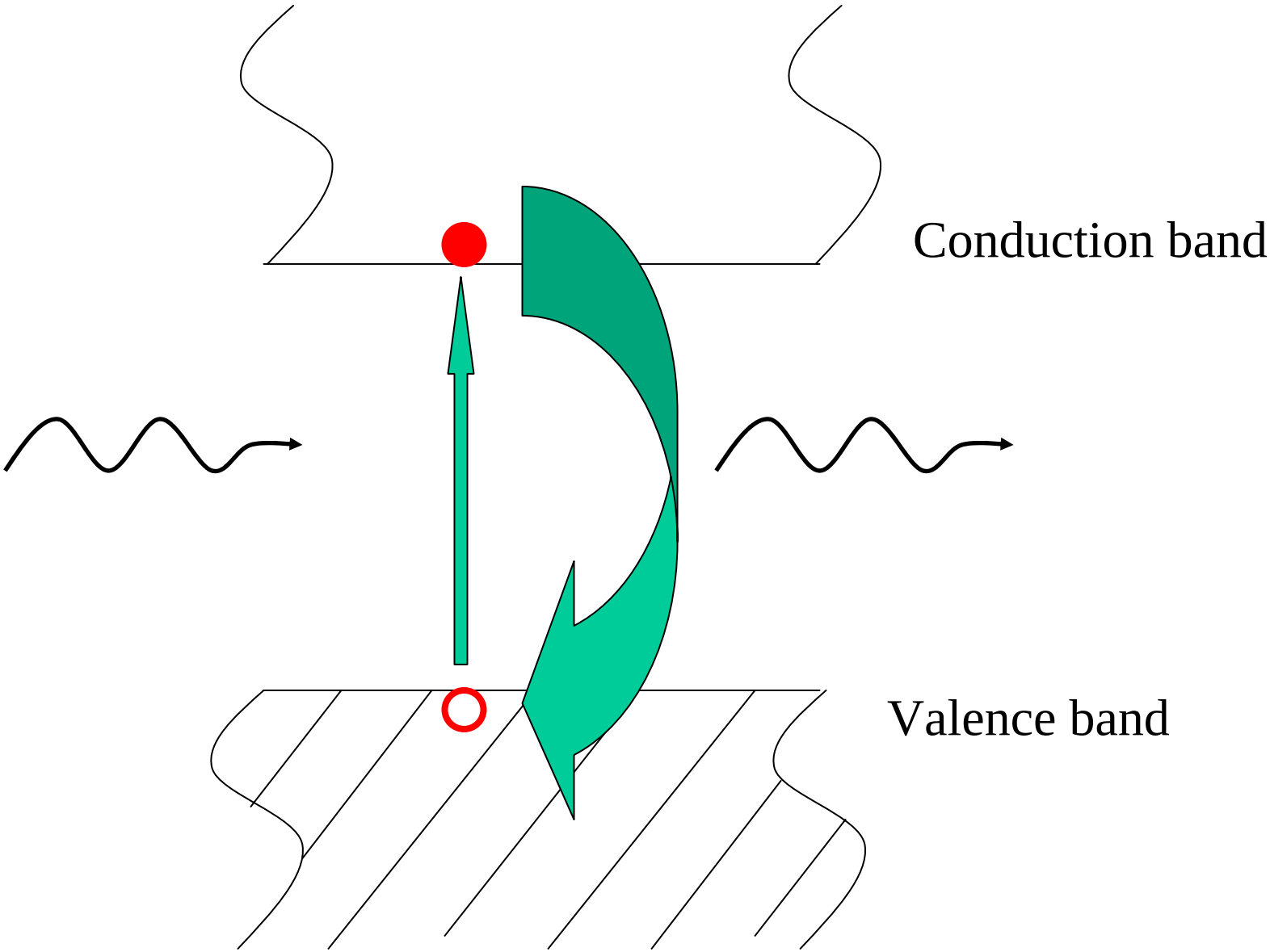
Sapra et al., J. Phys. D -Appl. Phys. 36 (2003) 1595

Bandgap variation in ZnO

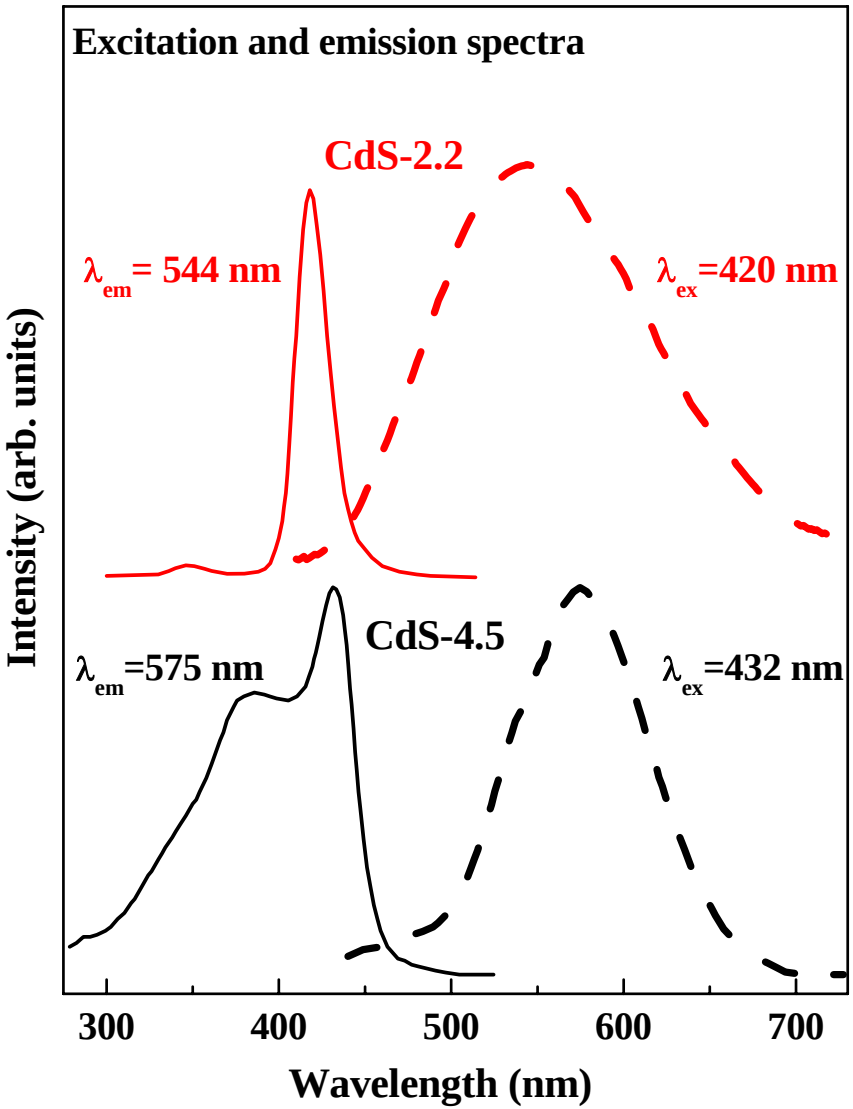


Viswanatha et al., J. Mater. Chem. (2004)

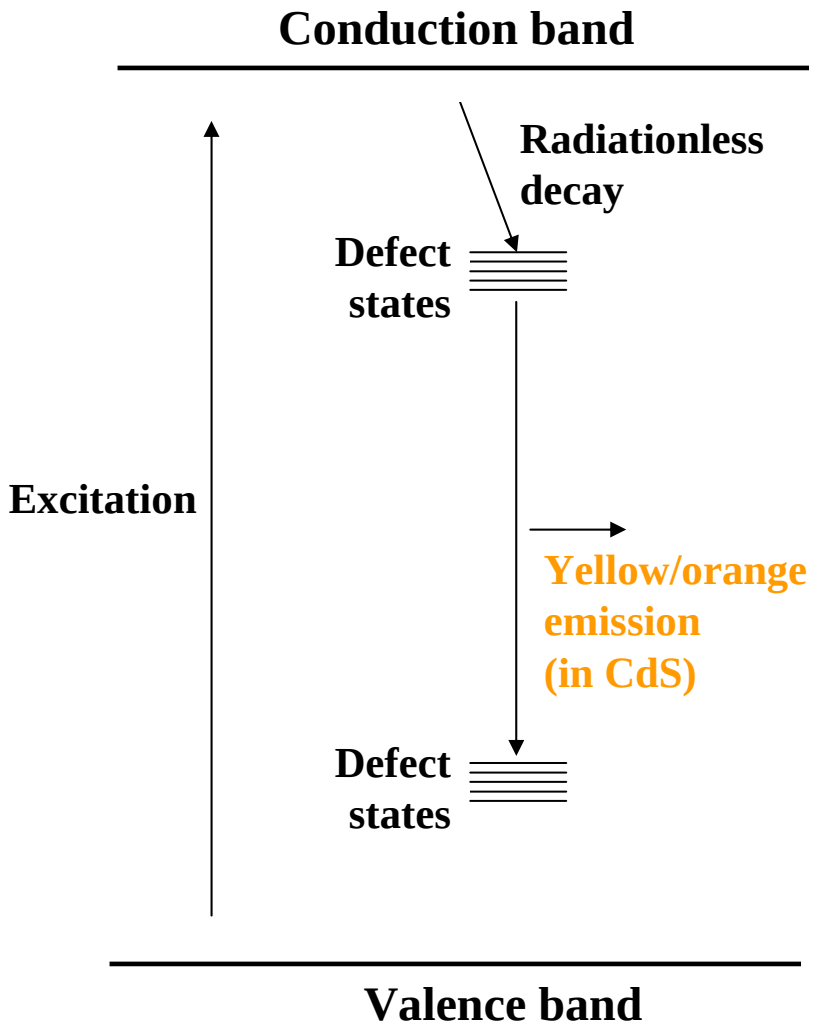
Let us get to the optical properties now



Emission spectra and surface states



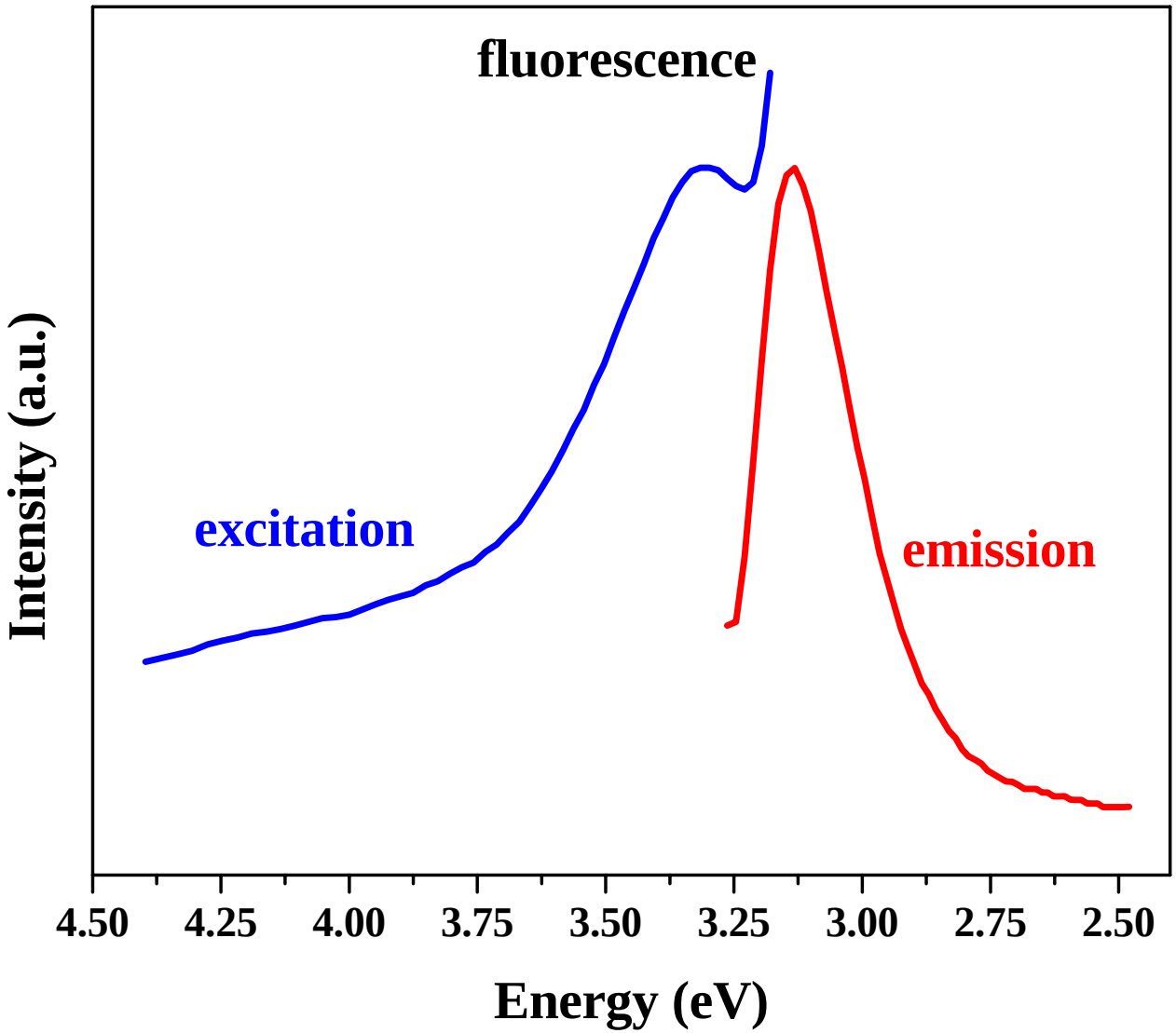
J. Nanda, Ph.D. Thesis, Bangalore



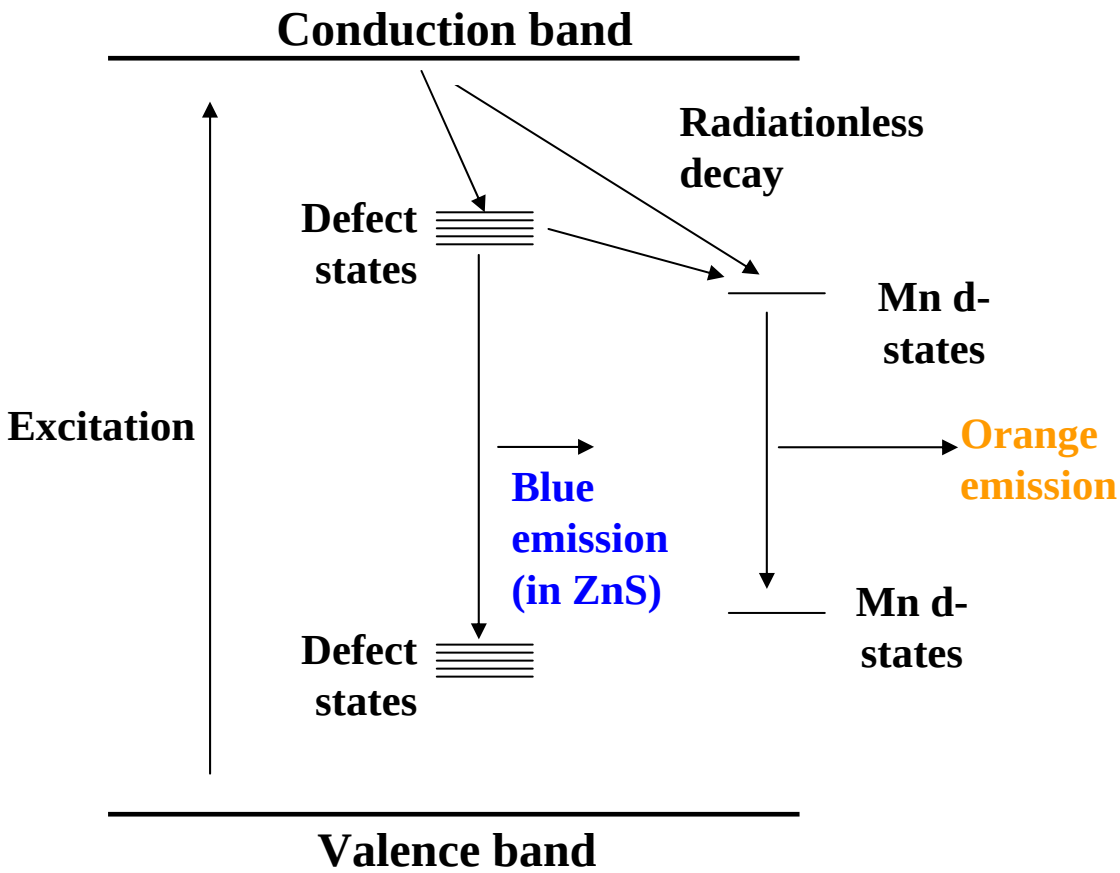
Blue emission from cysteine ester passivated cadmium sulfide nanoclusters,

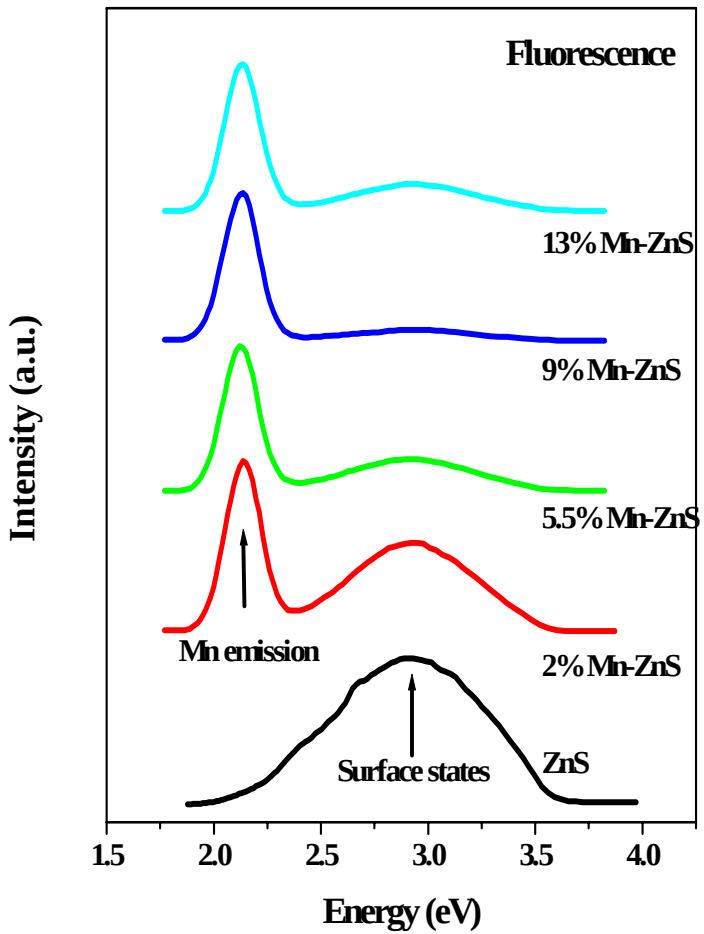
S. Sapra et al., Chem. Comm. 2188 (2001).

Band-gap emission from ZnSe quantum dots



Sapra et al. (preprint)

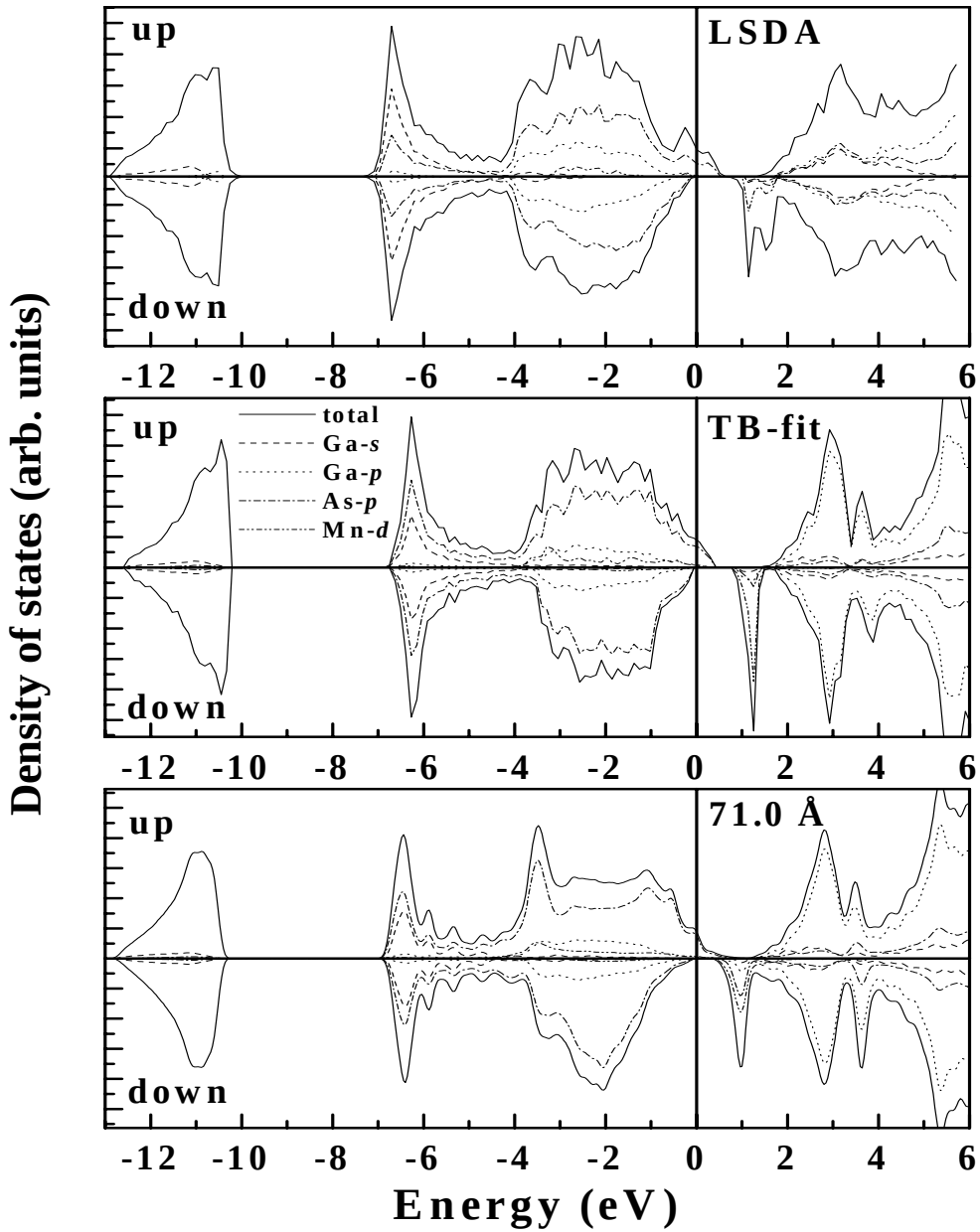




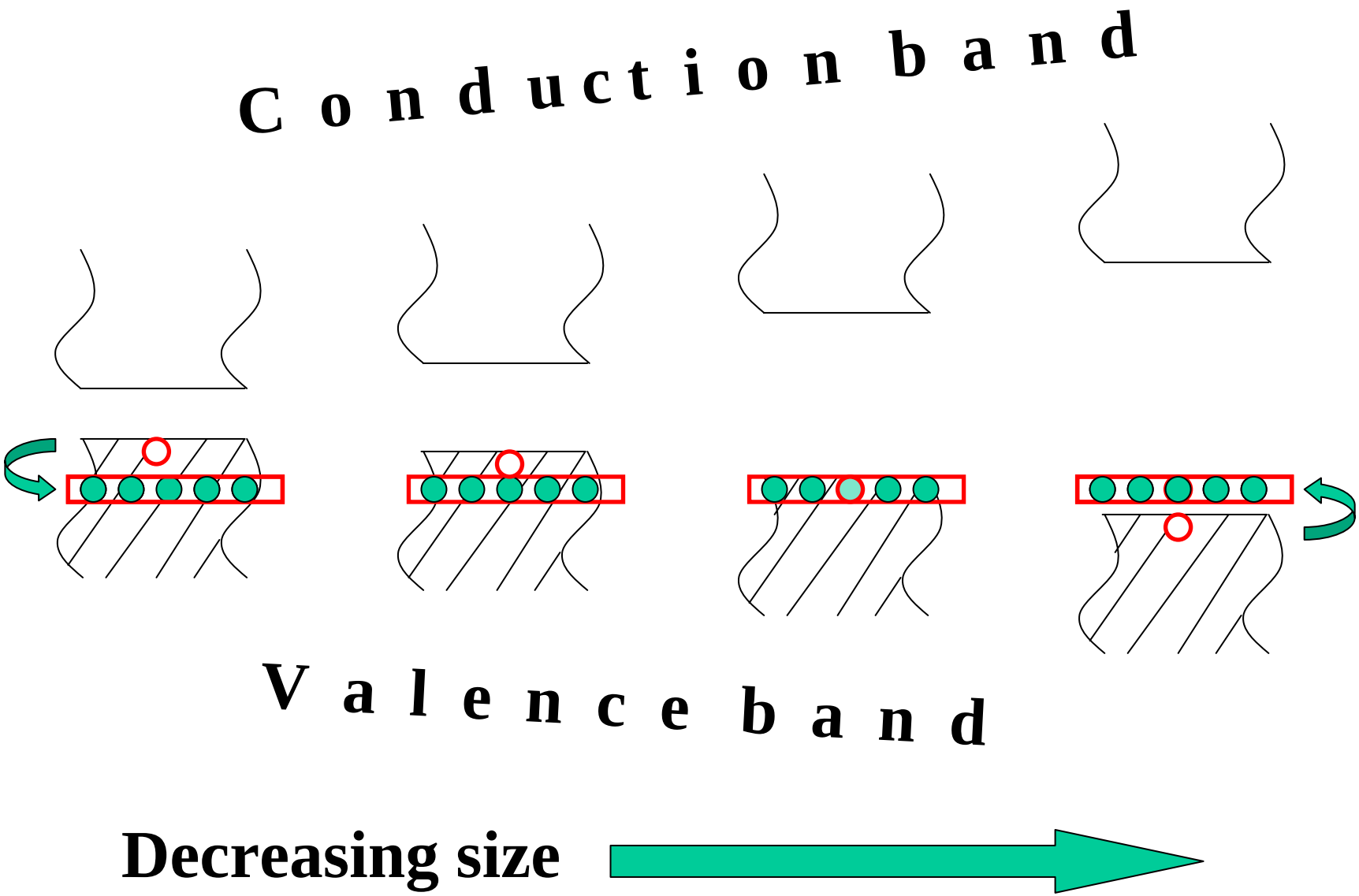
Sapra et al., J. Nanosci. Nanotech. (2003) and preprint.

Mn-doped GaAs: Bulk and cluster

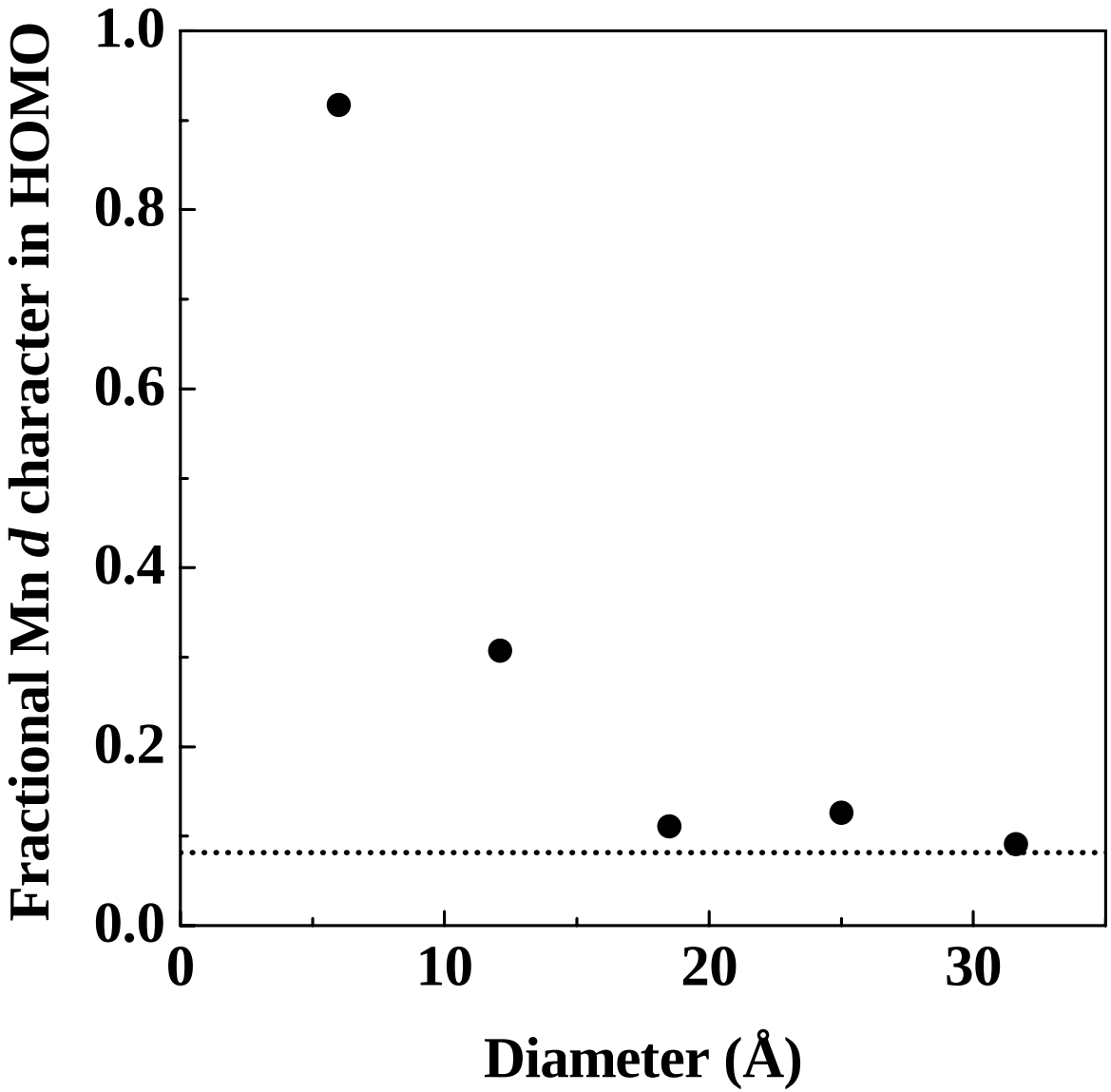
Issues in diluted magnetic semiconductors (DMS) nanoparticles.



Sapra et al., Nano Lett. 2 (2002) 605.


Conduction band
Valence band
Decreasing size

Mn-doped GaAs clusters



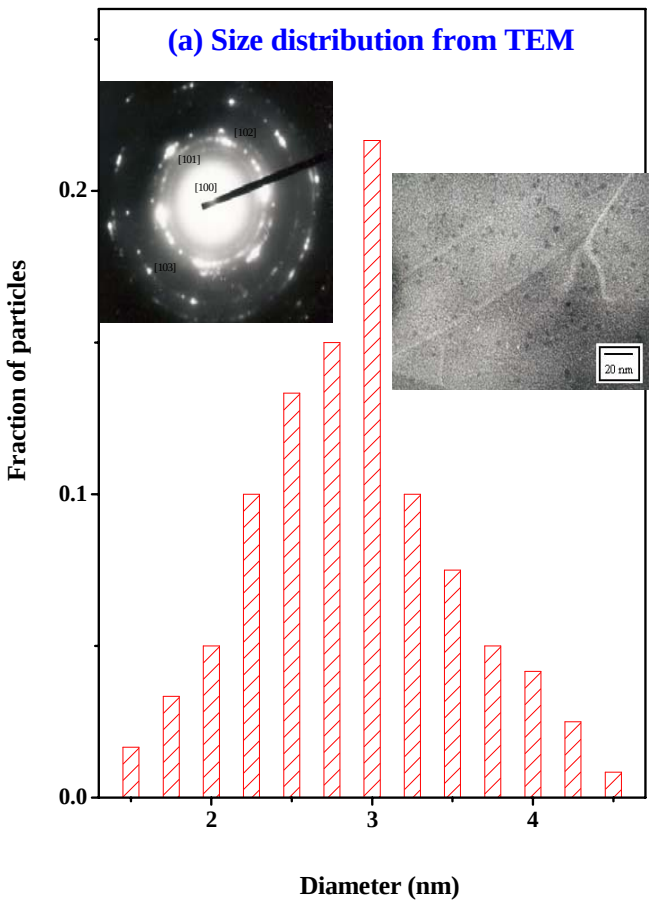
Suggestive of:

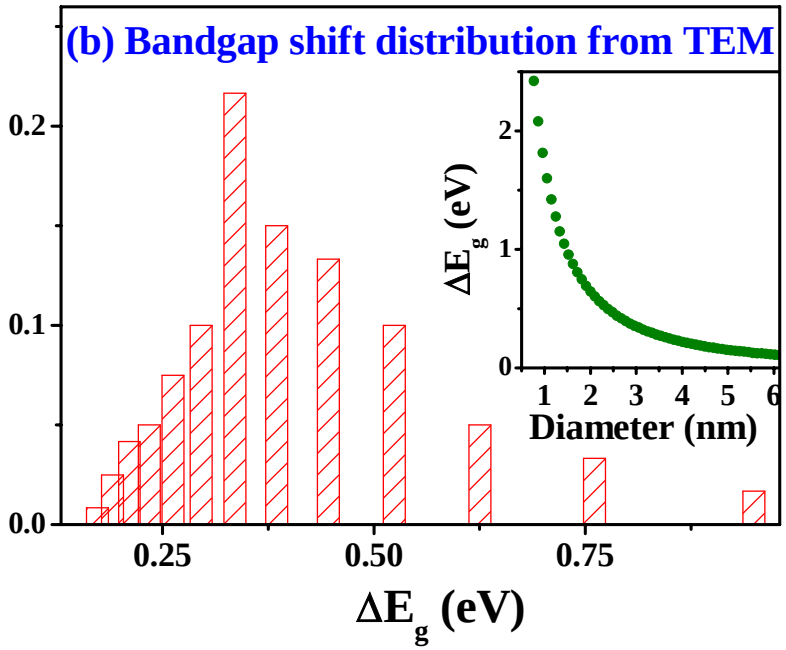
- Valence transition
- Electronic transition
- Magnetic transition

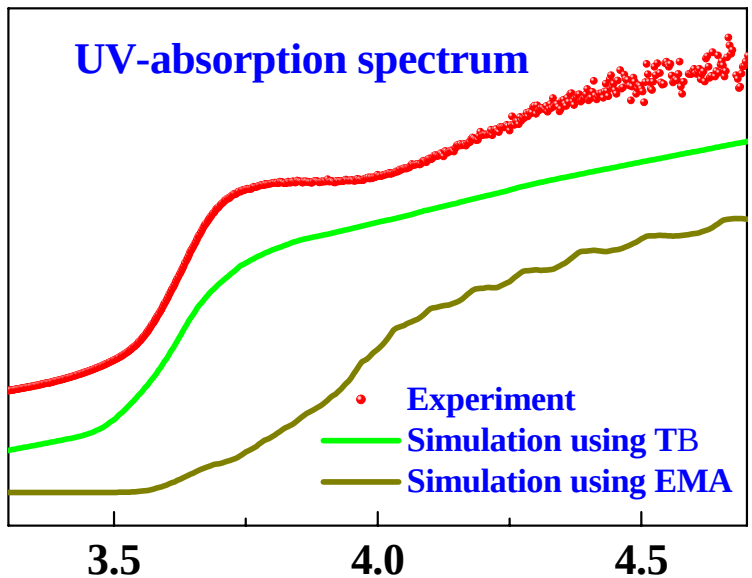
Sapra et al., Nano Lett. **2** (2002) 605;

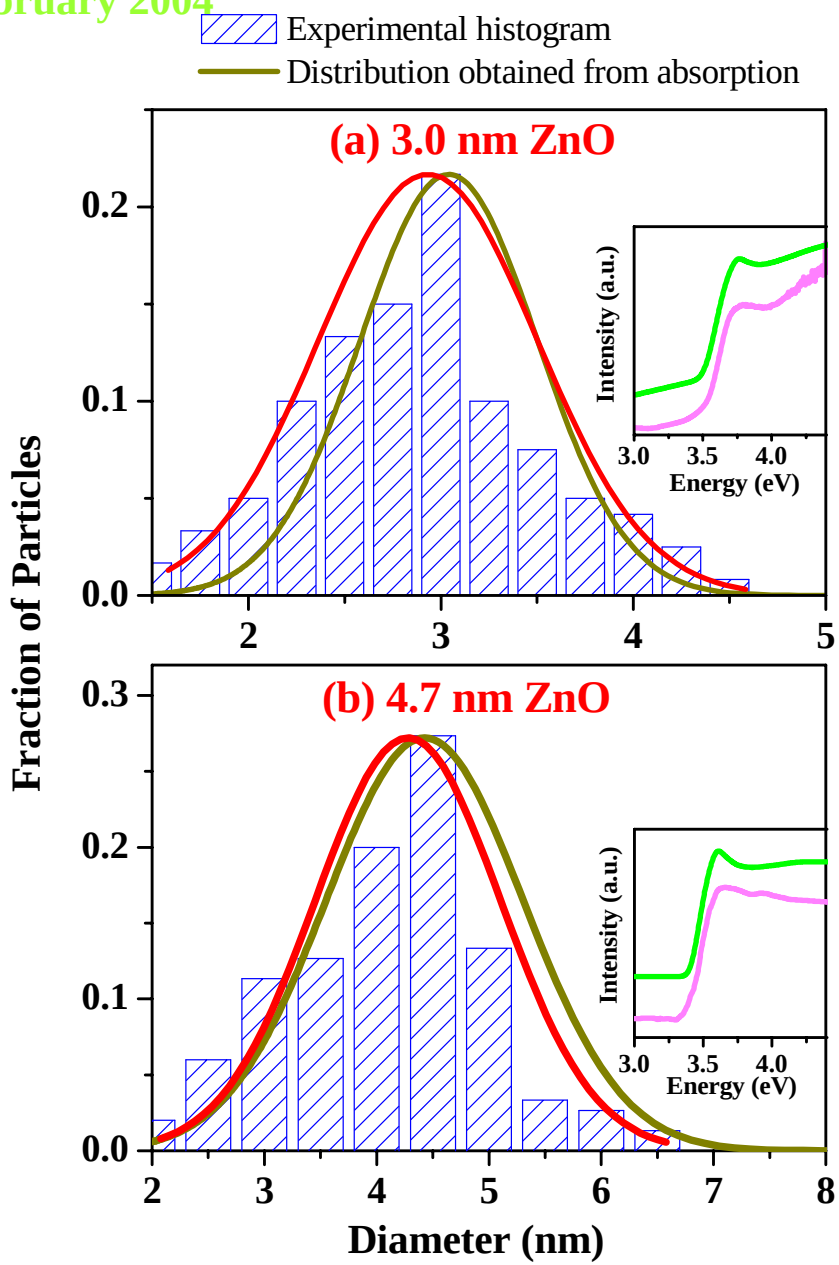
Also see Sarma et al., Phys. Rev. Lett. **85** (2000) 2549.

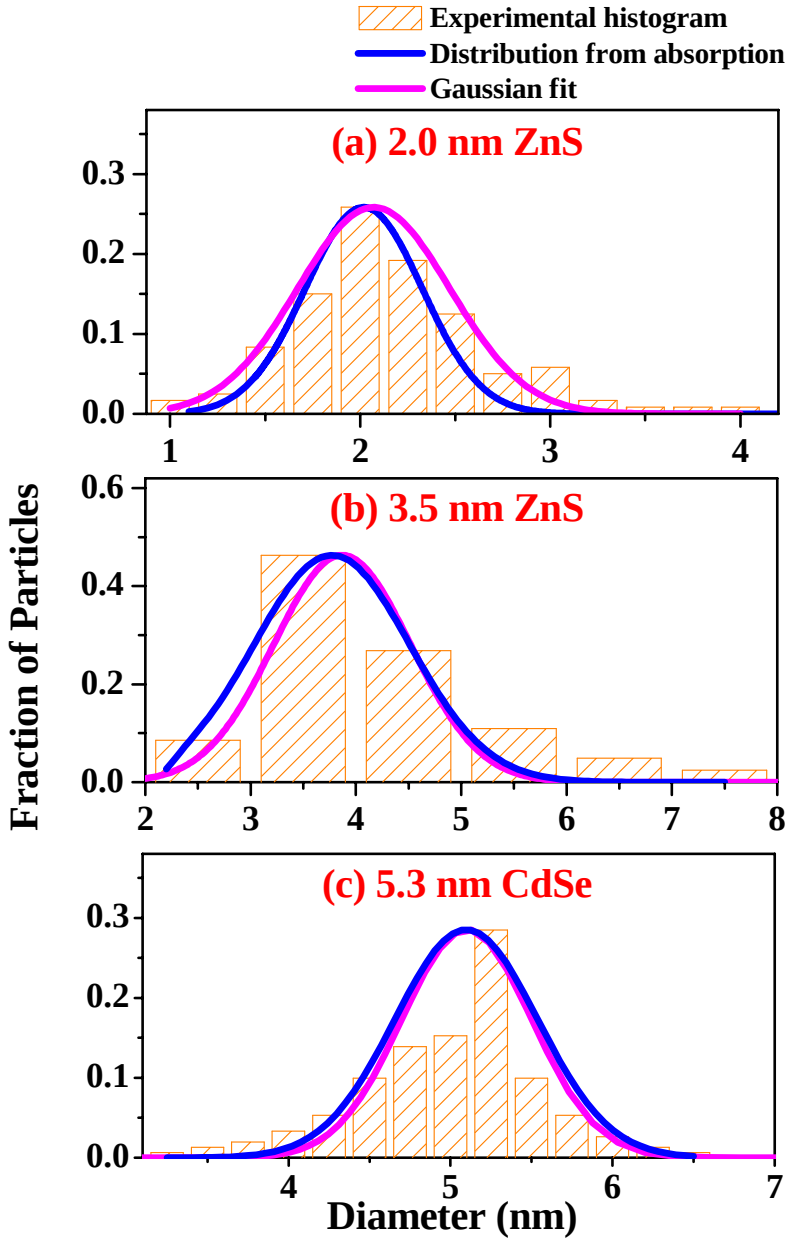
3.0 nm ZnO Nanocrystals

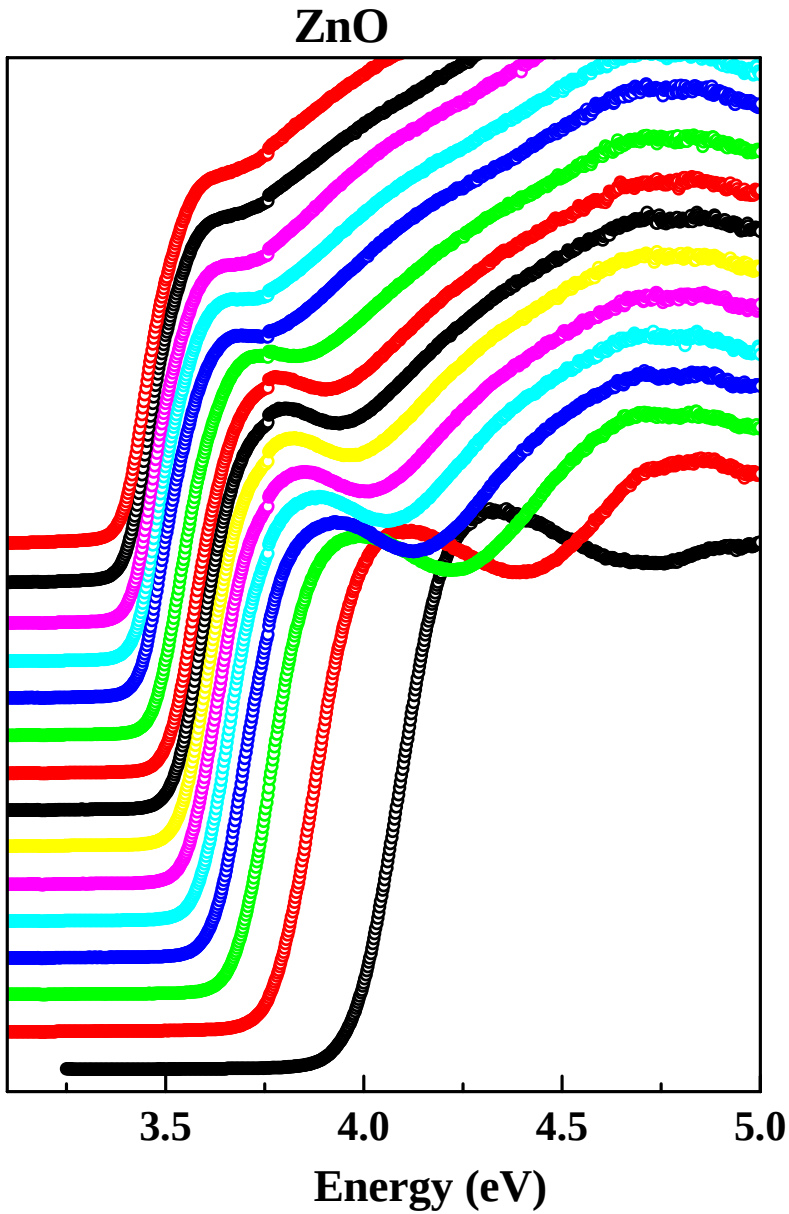


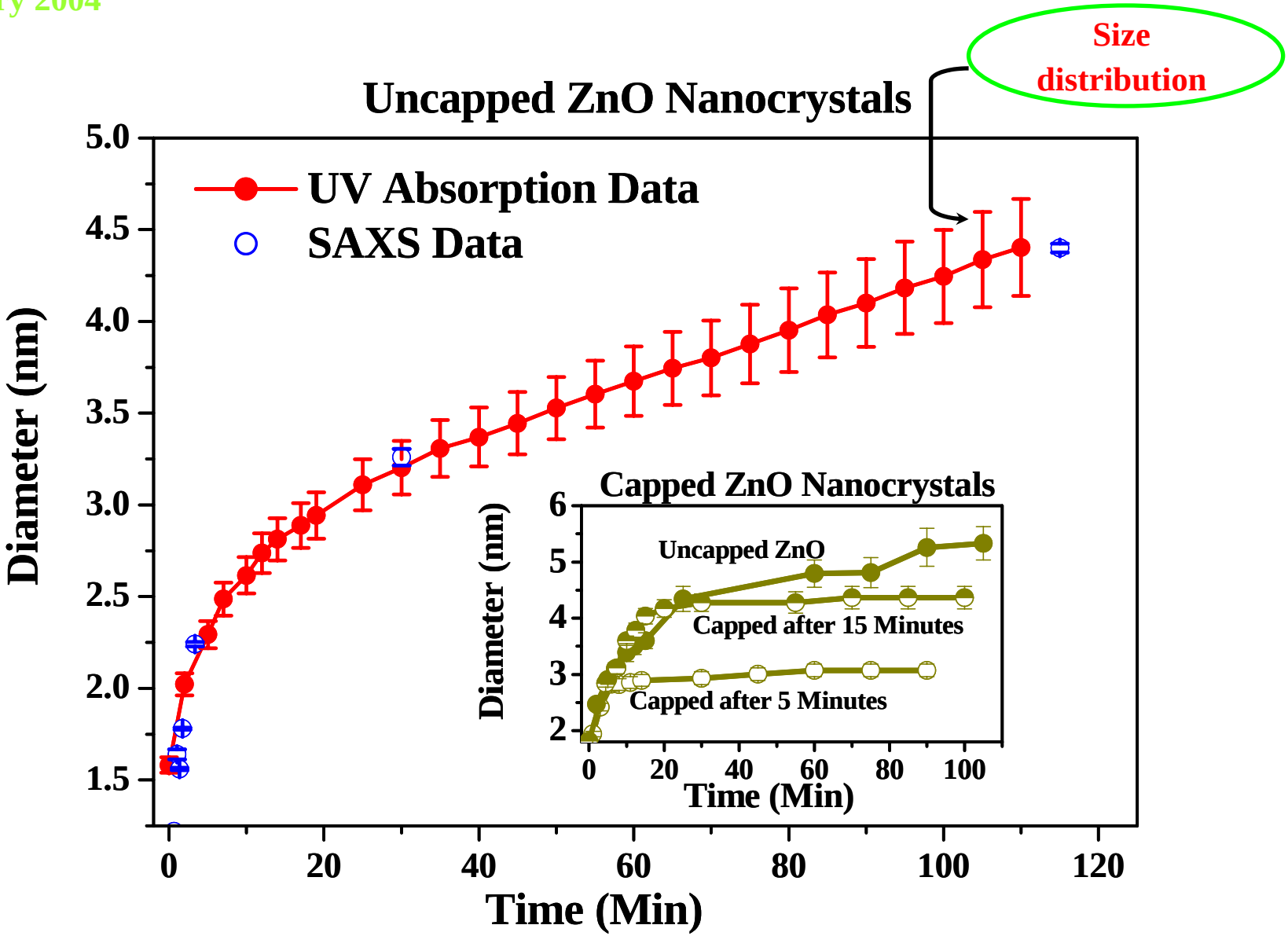





Experimental histogram
Distribution obtained from absorption
(a) 3.0 nm ZnO
(b) 4.7 nm ZnO
Intensity (a.u.)
Energy (eV)
Fraction of Particles
Diameter (nm)

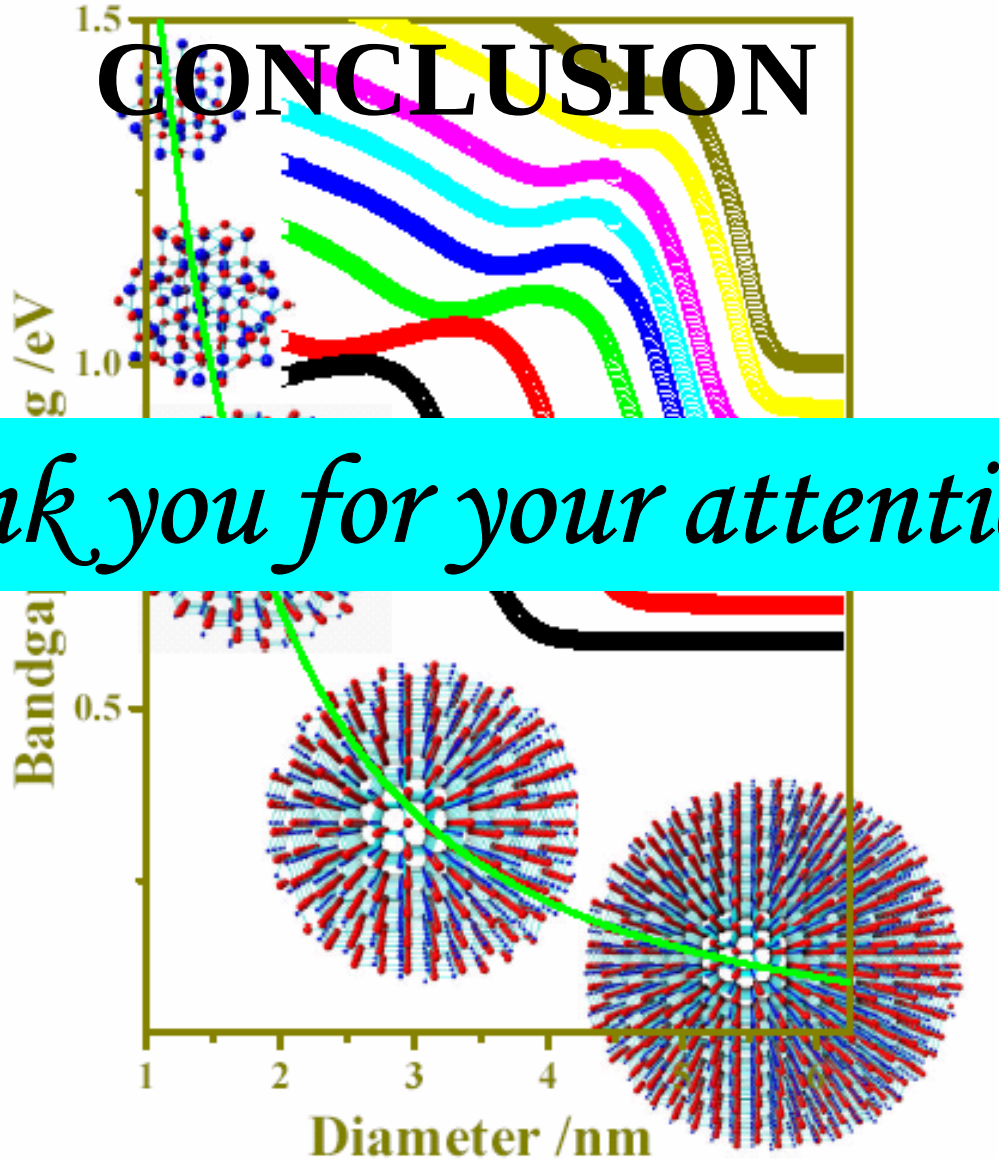

Experimental histogram
Distribution from absorption
Gaussian fit
(a) 2.0 nm ZnS
(b) 3.5 nm ZnS
(c) 5.3 nm CdSe
Fraction of Particles
Diameter (nm)


ZnO
3.5
4.0
4.5
5.0
Energy (eV)


Size distribution
Uncapped ZnO Nanocrystals
UV Absorption Data
SAXS Data
Diameter (nm)
Time (Min)
Capped ZnO Nanocrystals
Uncapped ZnO
Capped after 15 Minutes
Capped after 5 Minutes
Diameter (nm)
Time (Min)

CONCLUSION

GRAPHICAL SUMMARY



Experimental and theoretical demonstration of bandgap tuning in ZnO nanocrystals as a function of their size.

Thank you for your attention