COMSOL CONFERENCE STUTTGART 2011
OCTOBER 26-28

ISTITUTO ITALIANO DI TECNOLOGIA

Italian Institute of Technology

Super-Lattice Effects in Ordered Core-Shell Nanorod Arrays Detected by Raman Spectroscopy

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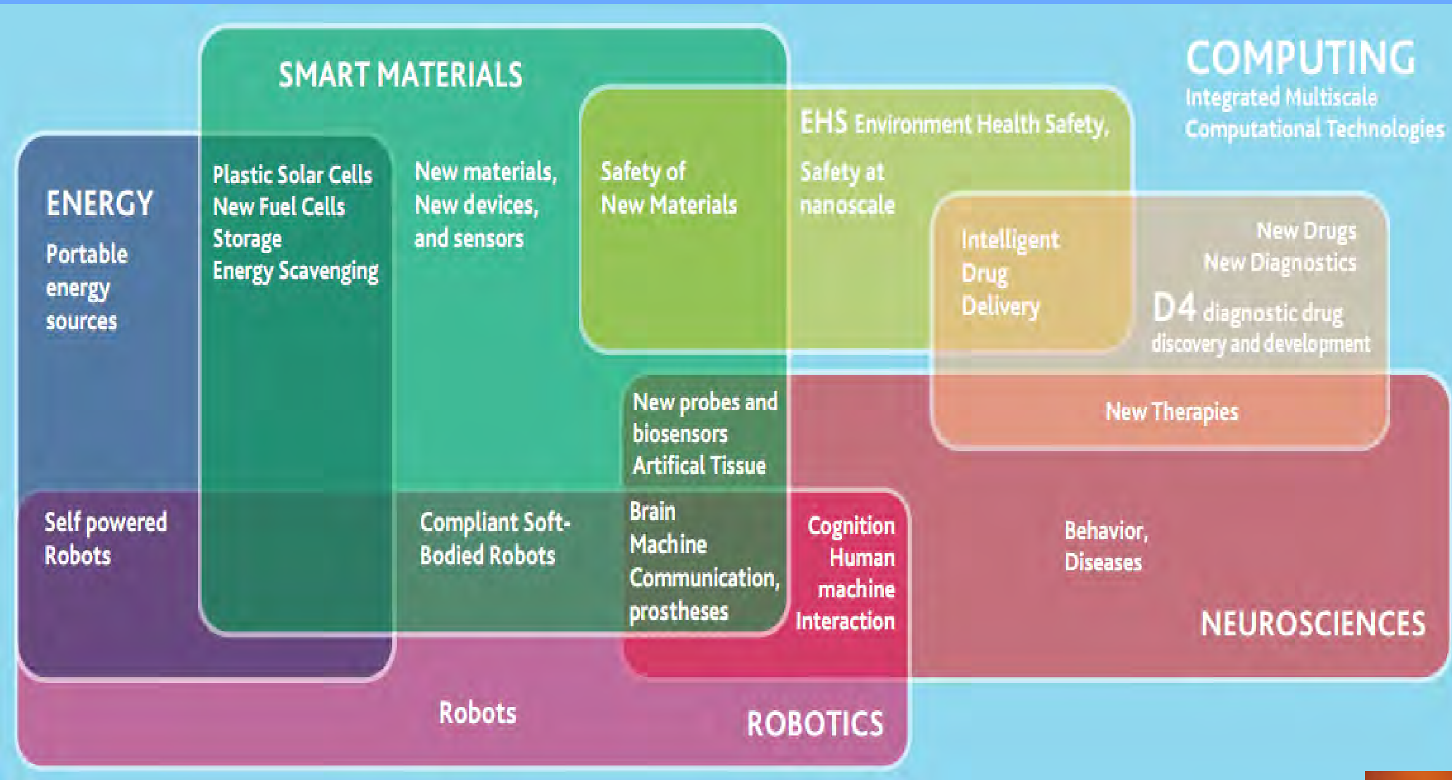
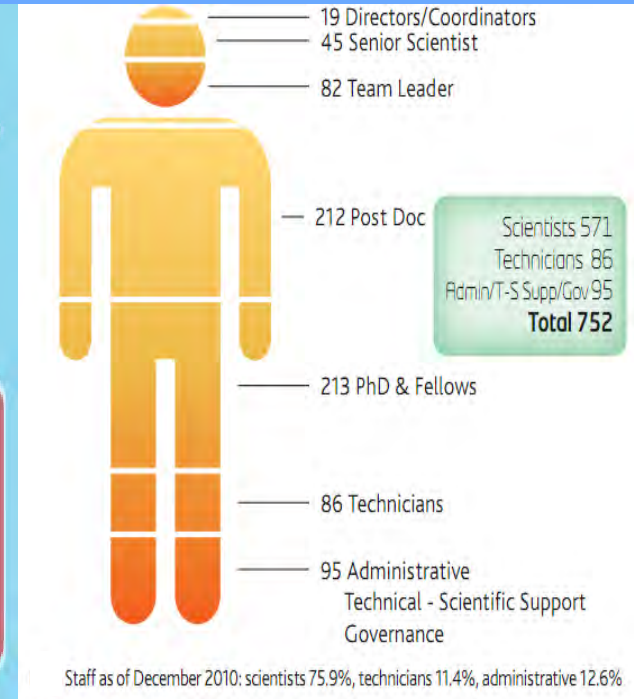
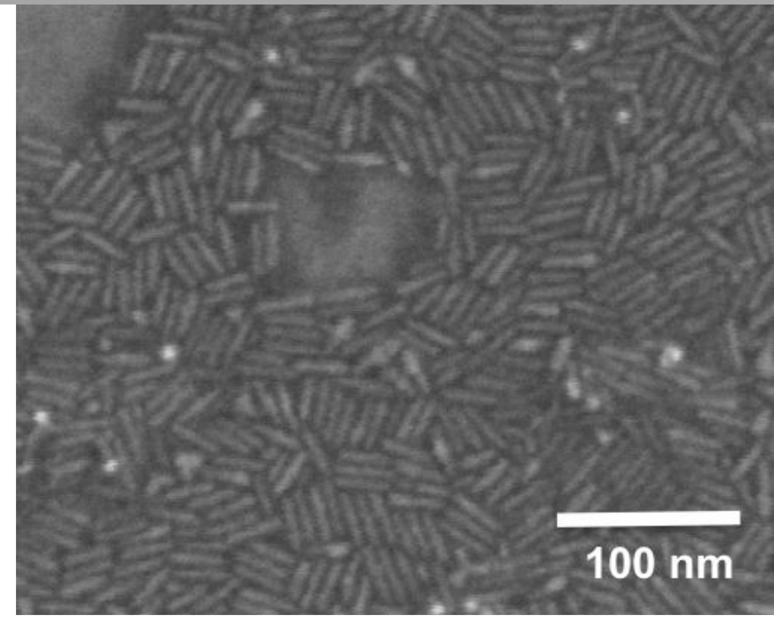




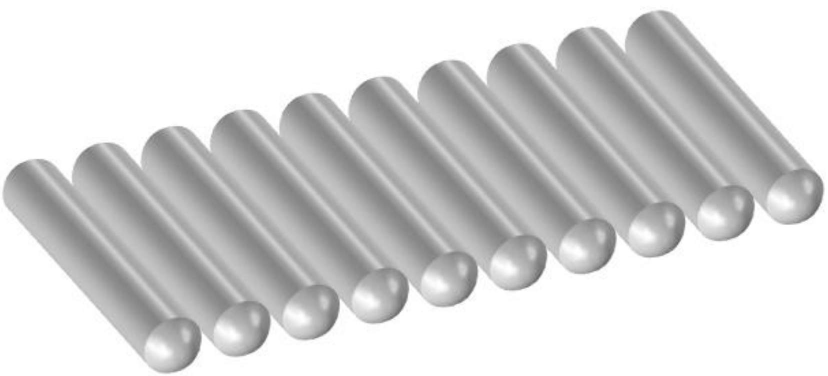
Ordered self-assembled nanocrystal promise novel physical properties due to collective effects and provide a cost effective way to fabricate macro-scale devices that rely on the peculiar properties of their individual components

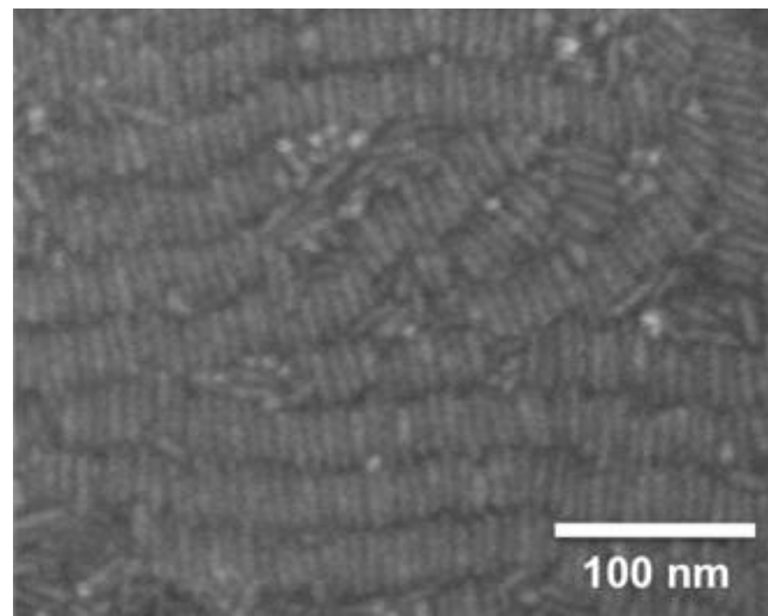
Why nanocrystals?

- Collective effects
- Cost effective way for macroscale devices
- Linearly polarized emission
- Orientation dependent conductivity



Arrays of dot/ rod core-shell CdSe/ CdS nanorods

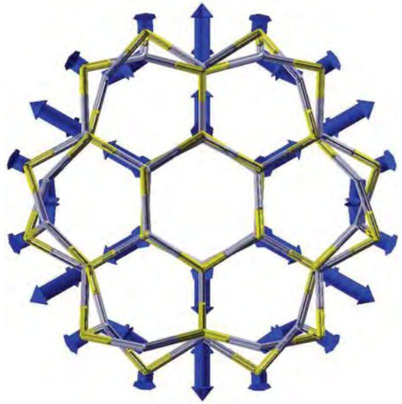




The vibrational modes (phonons) of nanocrystals can have significant impact on their optical and electrical response as manifested by phonon replicas in the emission spectrum

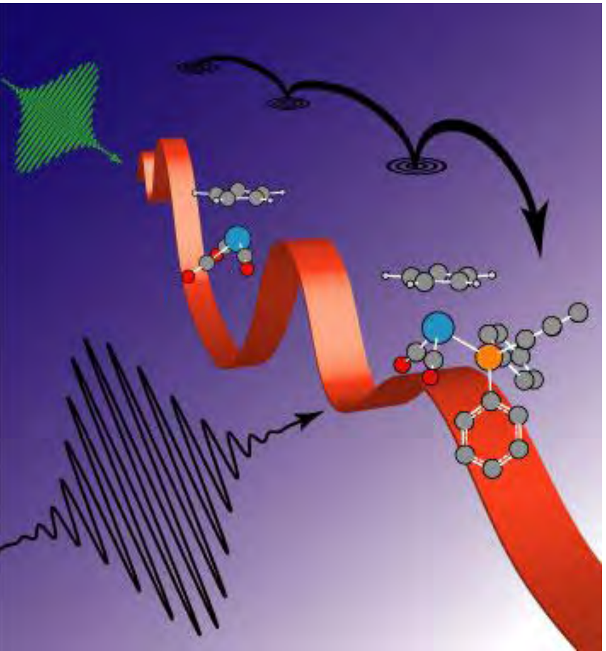
Nanocrystals and light

- Red-shift and broadening of longitudinal-optical (LO) phonon peak due to confinement effects
- Surface-optical (SO) phonon modes were found to depend on the aspect ratio of the nanorods



Calculated displacement pattern of the breathing mode of a 1.4 nm diameter CdSe nanowire

H. Lange *et al.* Nano Lett. (2008)

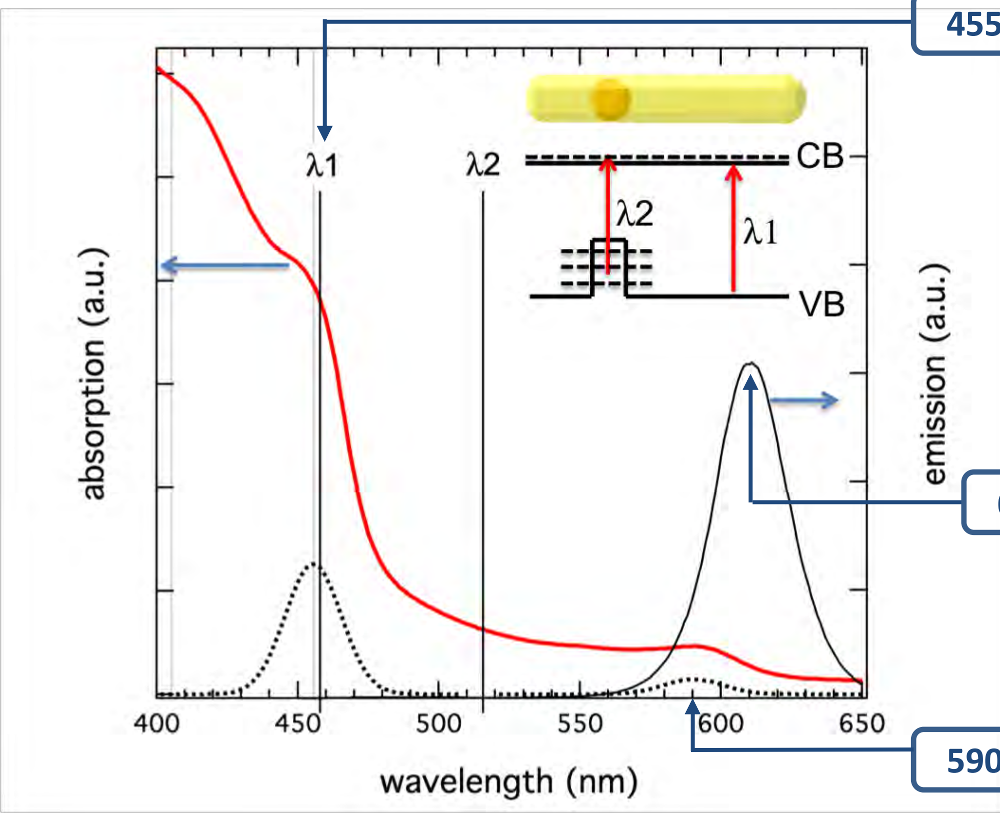


- Radial breathing modes have been observed both in spherical and rod-shaped nanocrystals
- Linearly polarized Raman experiments on oriented arrays of CdSe nanorods allowed to distinguish LO phonon modes oscillating parallel and perpendicular to the nanorod axis

In this work we report Raman experiments on core-shell CdSe/CdS nanorods with a dot-in-a-rod architecture that self-assembled into micron size tracks

Characterization of CdS/CdSe nanorods

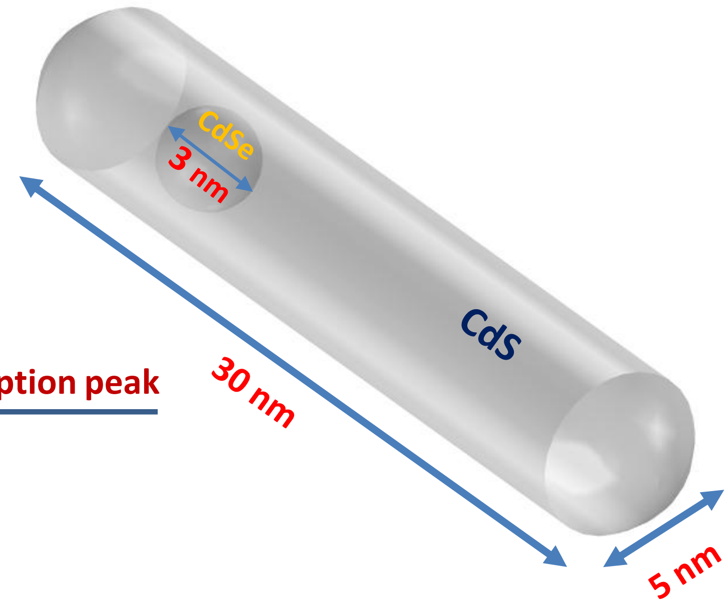
Optical Absorption and Emission spectra



455 nm CdS absorption peak

610 nm CdSe emission peak

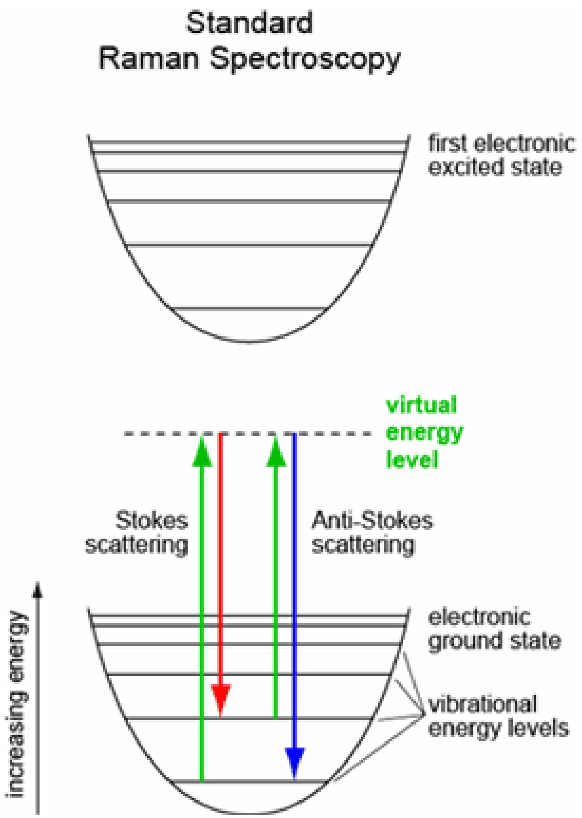
590 nm CdSe absorption peak



The emission peak at 610 nm is red-shifted with respect to the CdSe core absorption due to the Stokes shift

At the excitation wavelength λ1=458 nm the Raman signal is in resonance with the transitions in the nanorod shell (CdS), while at λ2=514 nm it is in resonance with transitions related to excited states in the CdSe core

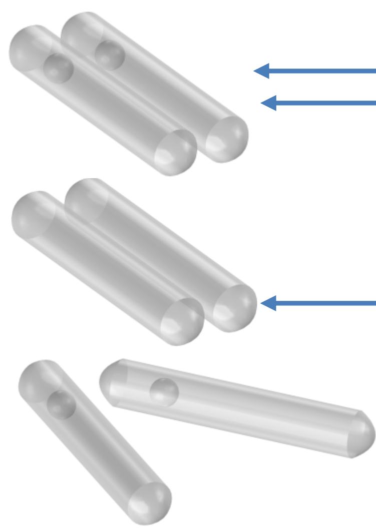
Raman spectroscopy on nanorods' tracks



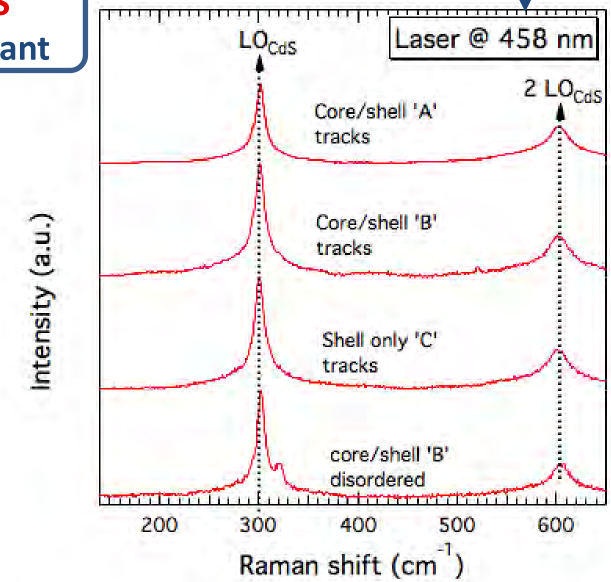
Broad Raman peak at 295 cm^{-1}

Only observed if:

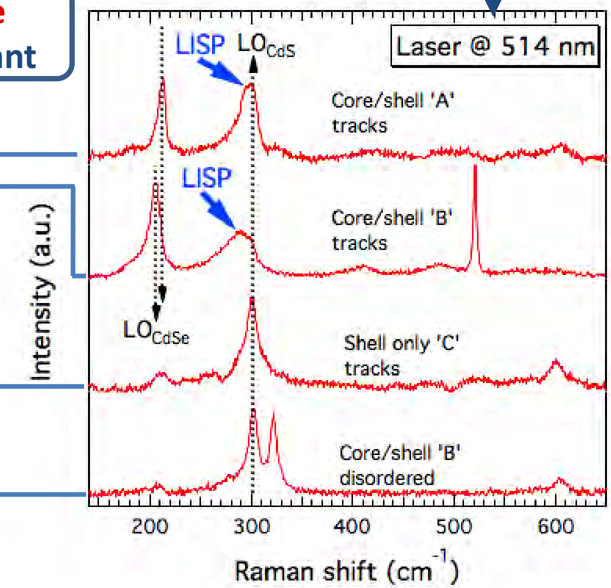
- Nanorods are assembled into a **superlattice**
- Excitation wavelength in **resonance** with the excited **states of the CdSe core**



CdS resonant

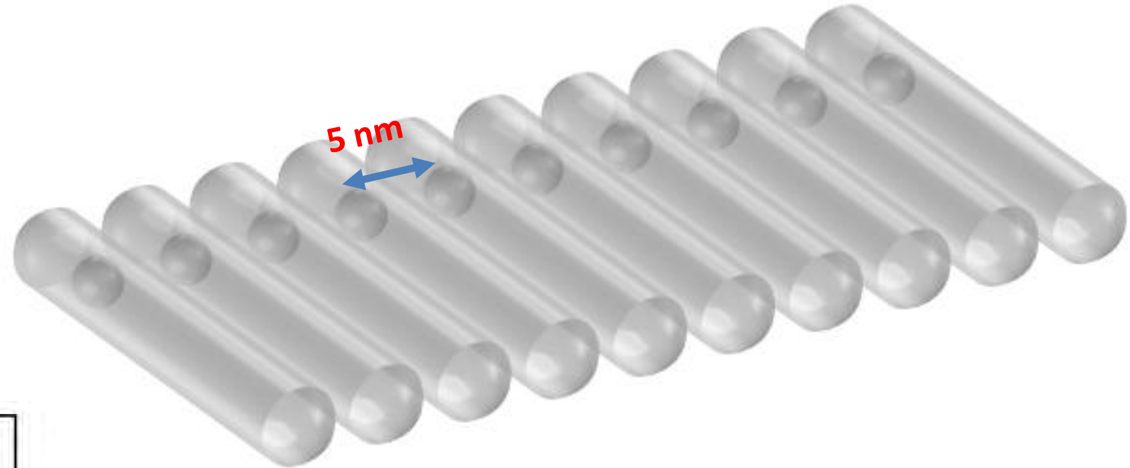


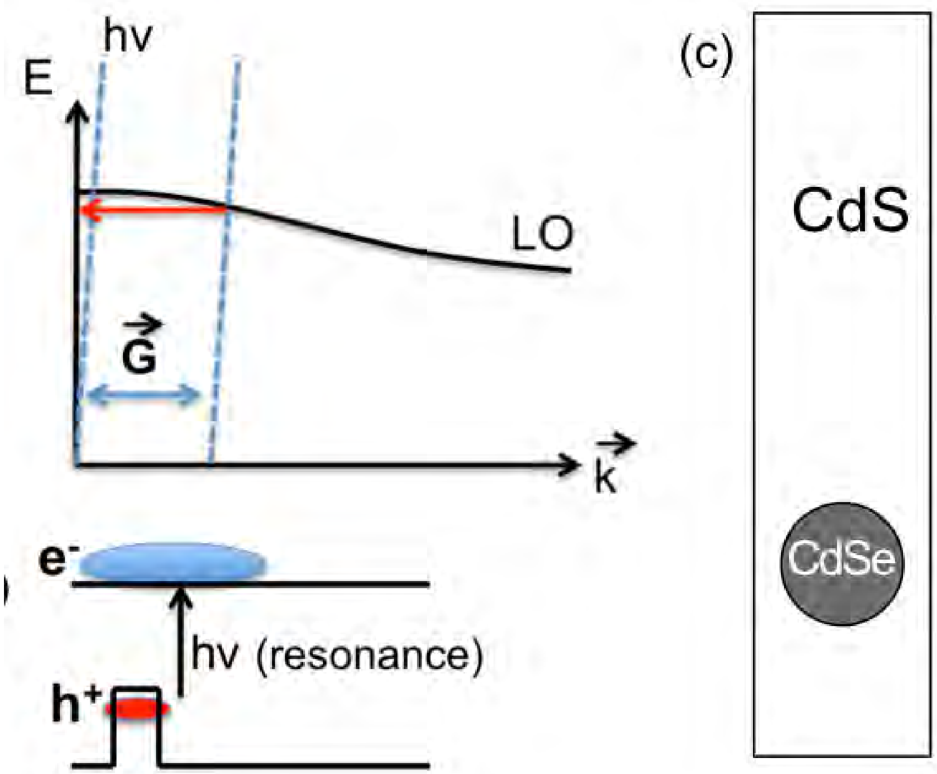
CdSe resonant



The broad LISP peak was in resonance with electronic transitions of the CdSe core. Since this mode is only observed in spectra from the nanorod tracks, we can attribute its origin to a super-lattice effect

Proposed grating coupling effect

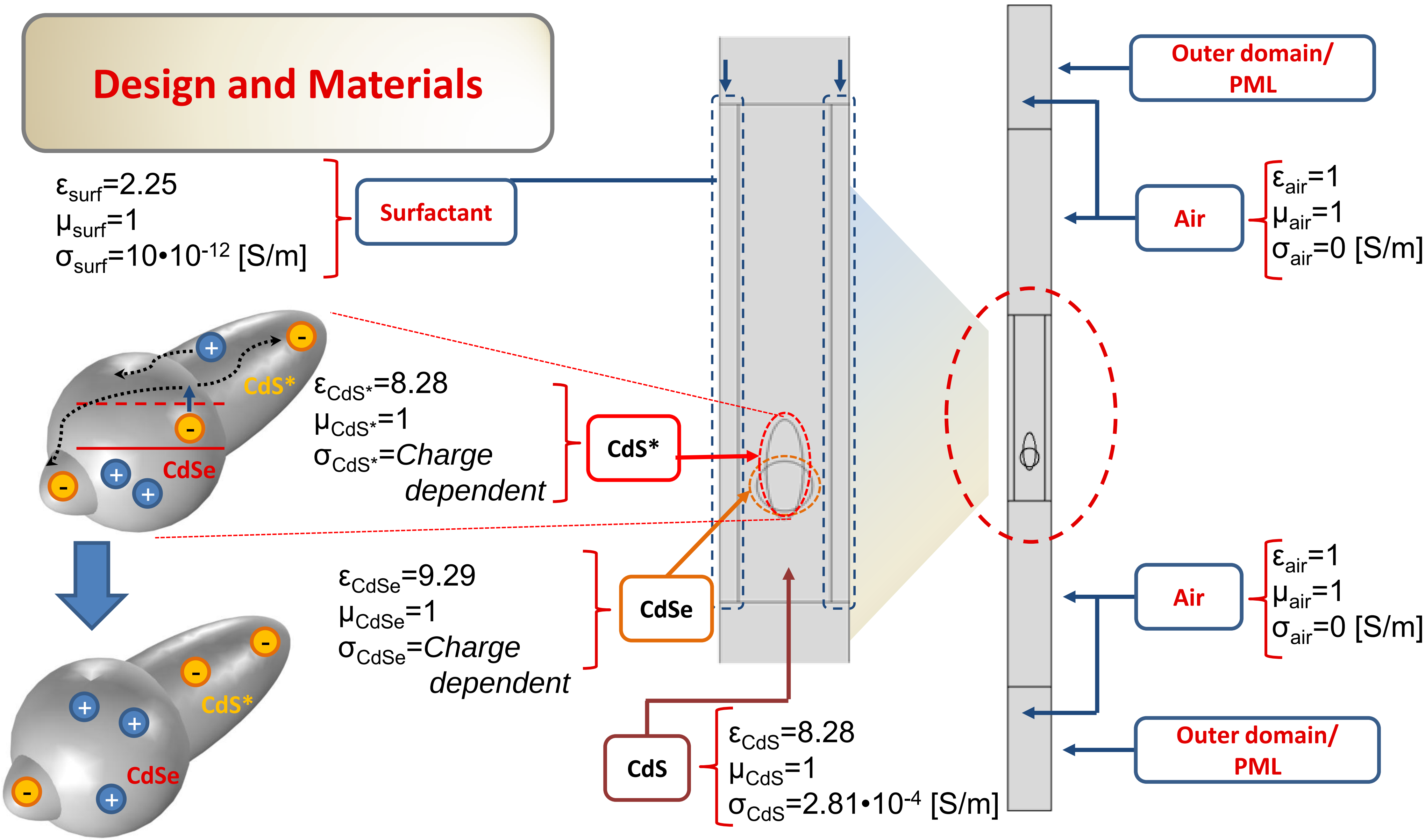




We propose that a grating coupler effect is produced by photo-induced charges localized in the vicinity of the CdSe cores

Our 2D COMSOL model assumed the charge distribution of the photo-generated electrons was approximated by an elliptical area, and the holes were confined in the spherical CdSe core region

Design and Materials

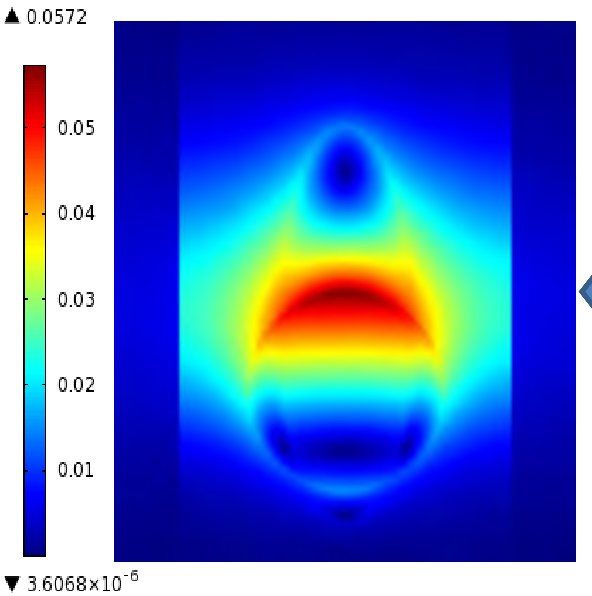


Localized charges have been set-up to mimic the promotions of electrons and an electrostatic simulation was launched. The resulting displacement field **D** has been used to modify material parameters for electromagnetic interactions

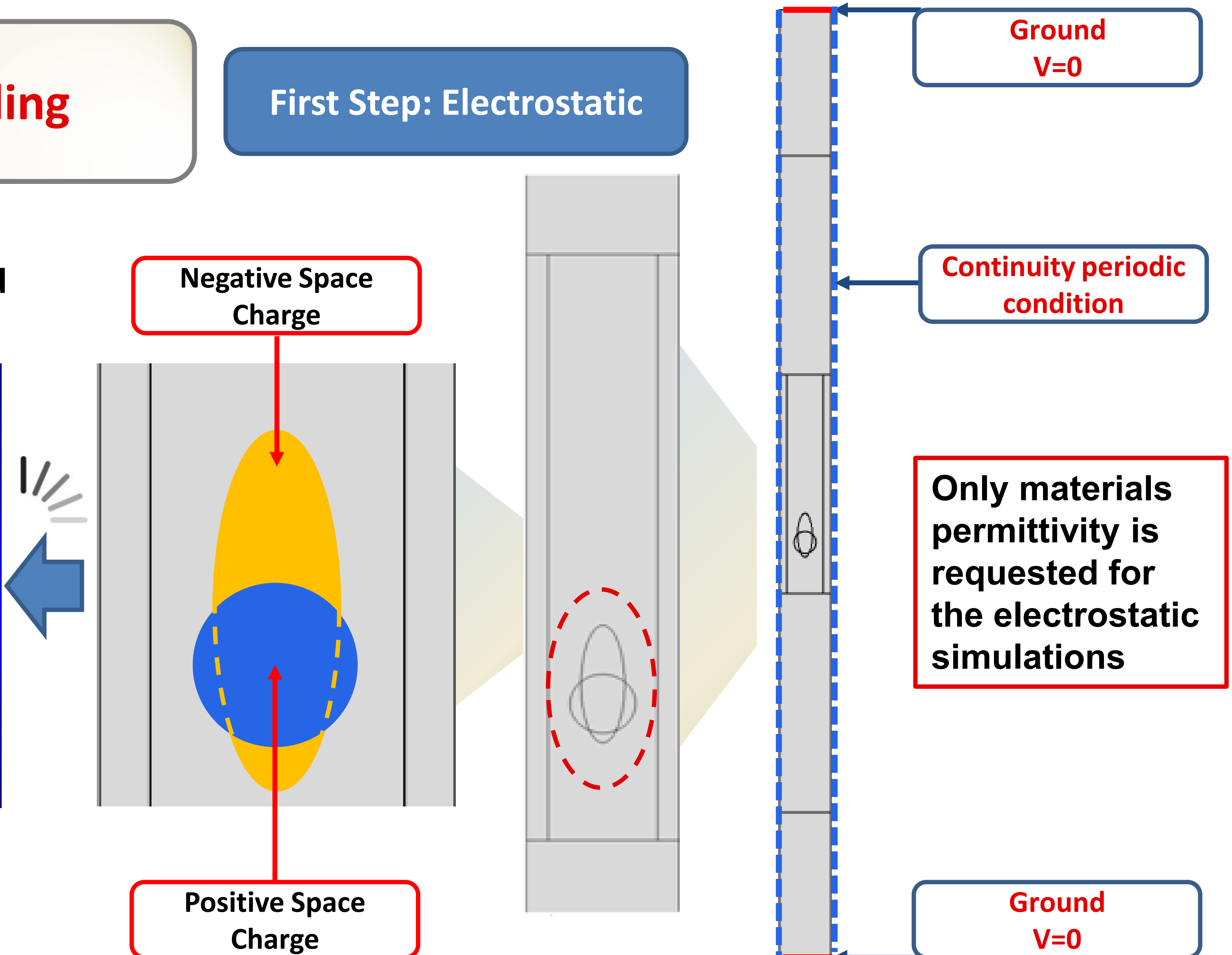
Physics modeling

First Step: Electrostatic

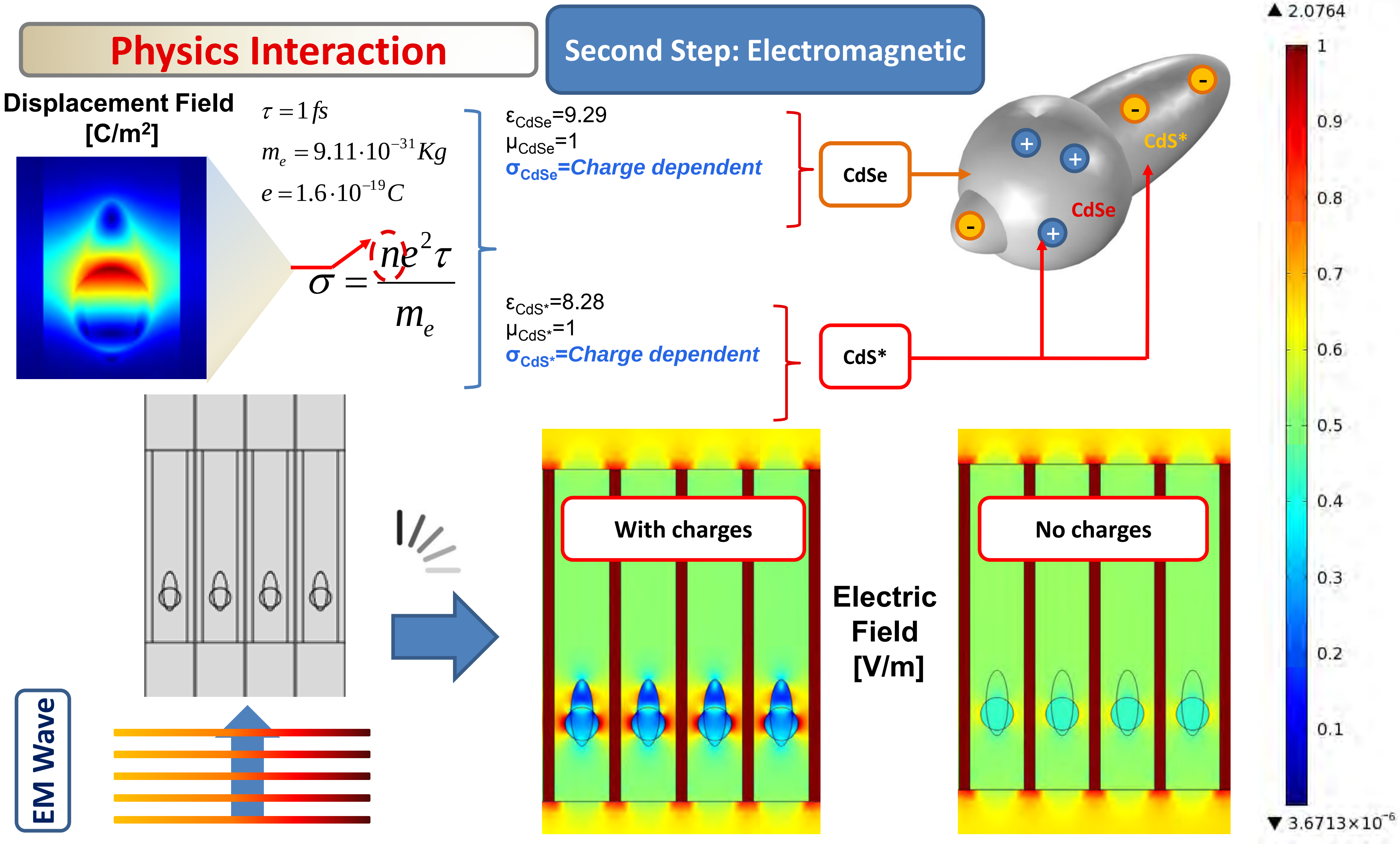
Displacement Field [C/m²]



$$\begin{cases} \nabla \cdot \vec{D} = \rho \\ \vec{E} = -\nabla V \end{cases}$$

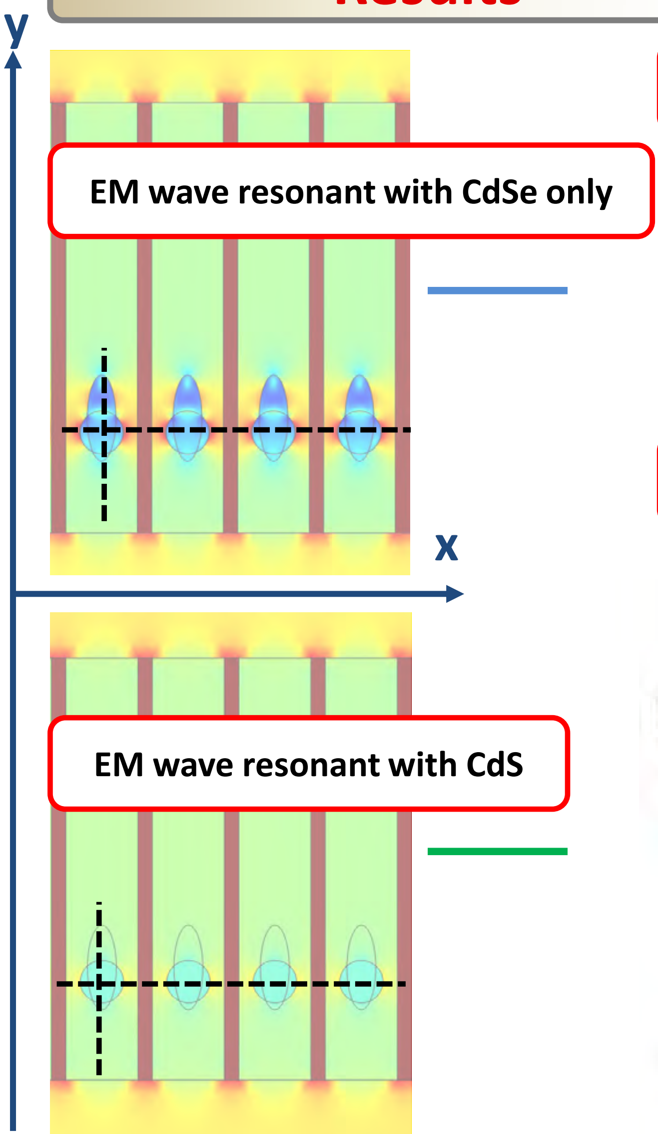


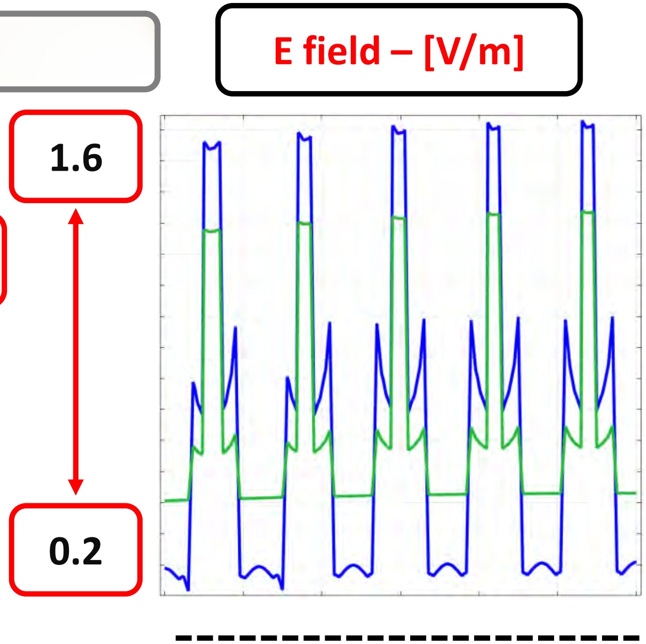
The calculated electric displacement modifies CdSe and CdS* conductivity and thus the interaction with the impinging electromagnetic wave

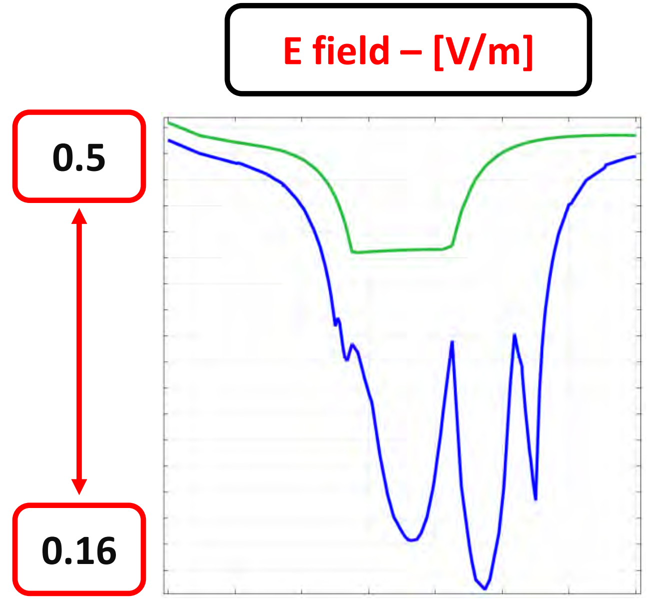


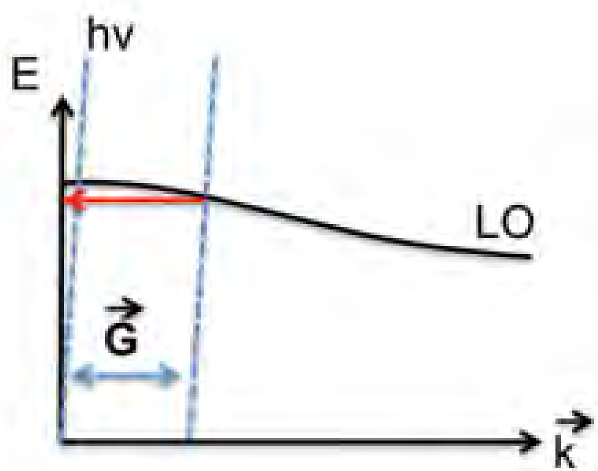
We have calculated with COMSOL the magnitude of the electric field vector E of a plane electromagnetic wave polarized in x-direction and traveling in y-direction at a wavelength of 514 nm in an array with, and without, localized charges

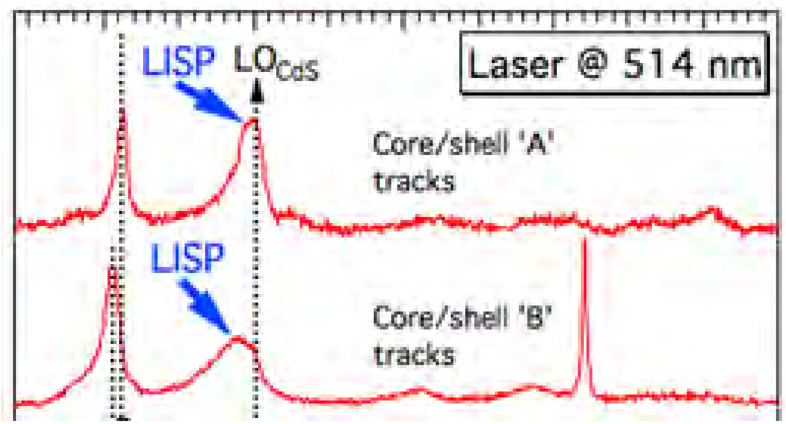
Results



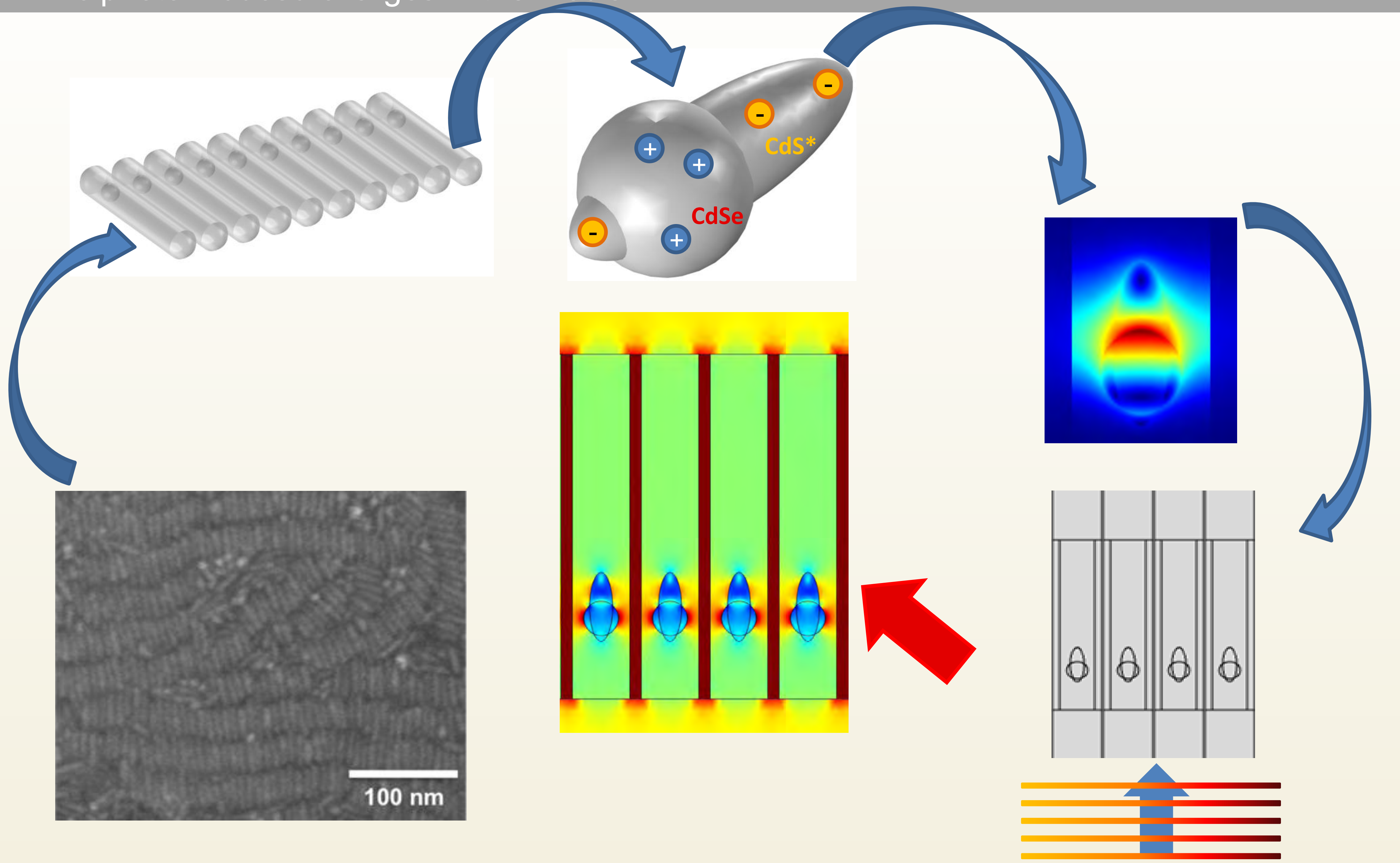








Starting from experimental results we modeled and calculated the interaction of an electromagnetic wave with our system combining electrostatics and electrodynamics to mimic photo-induced charges in the media



Thank you for your attention