Band Structure and Impurity Effects on Optical Properties of Quantum Well and Quantum Dot Infrared Photodetectors

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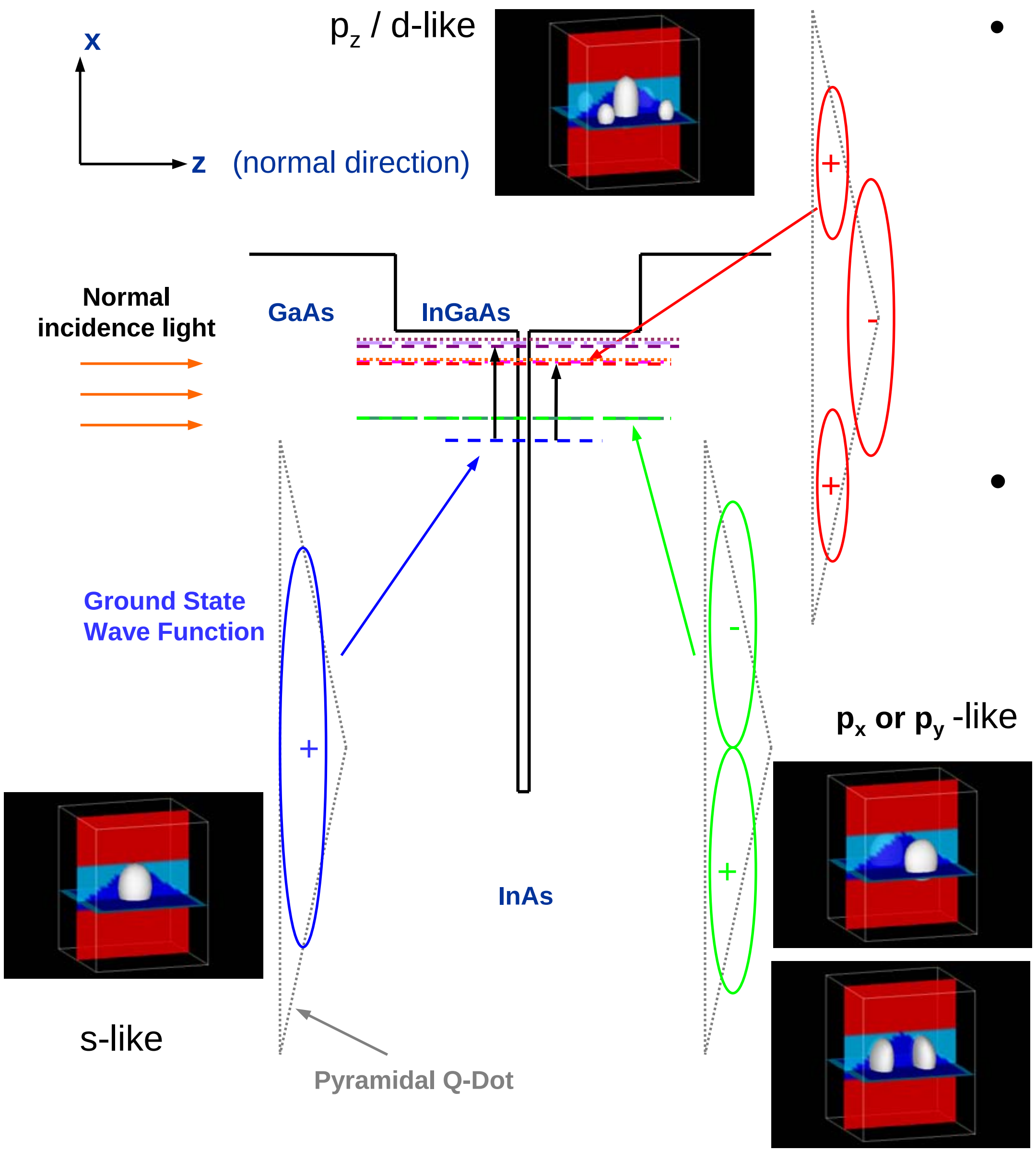
Motivation and Approach

- Experimentally measured photoresponse of an InAs/InGaAs/GaAs dot-in-the-well (DWELL) structure shows normal incidence response can be a sizeable fraction of the 45° incidence response.
- Experimentally measured photoresponse of an AlGaAs/GaAs/AlGaAs QWIP structure shows sizeable backgroud absorption at long wavelengths (>10μm)
- Explore this physical phenomenon by theoretical investigation (14-band model + impurity) for possible explanations.

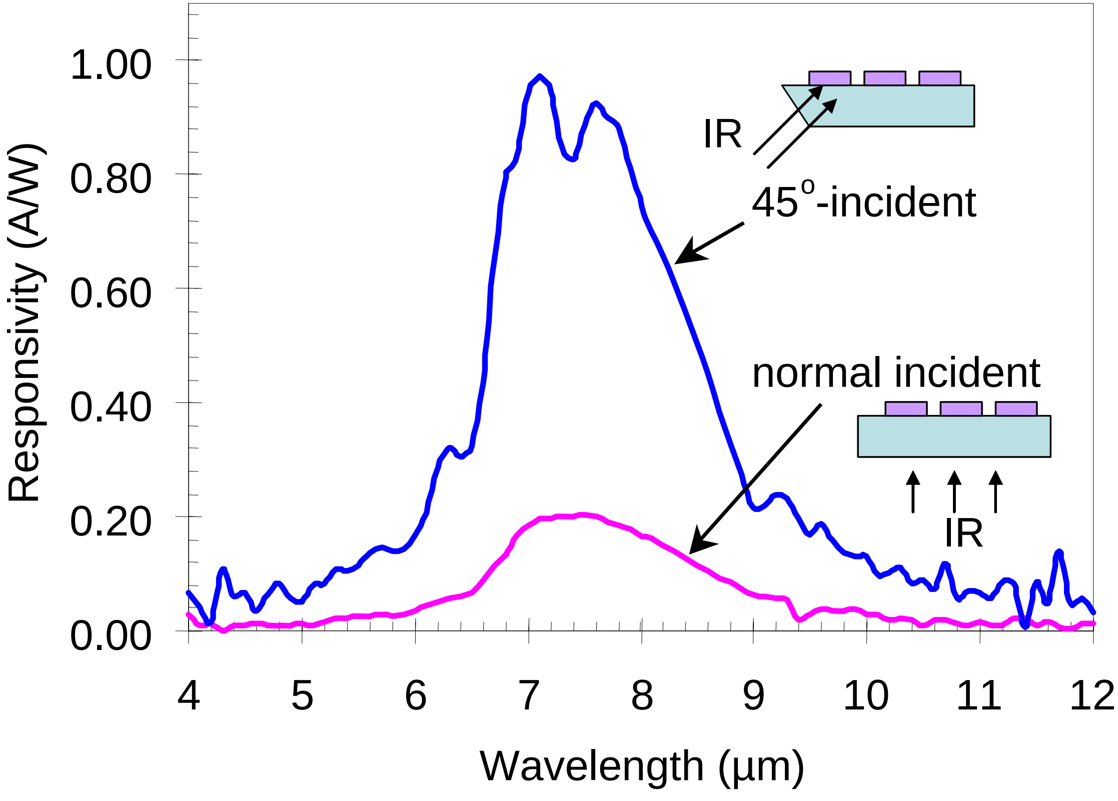
Photoresponse in DWELL Structure



- The fundamental transition (ground to p_x or p_y like states) yields no appreciable photocurrent.
  - Very strong normal incidence absorption.
  - But upper state is deeply bound

- Observed photocurrent is attributed to transitions from the s-like ground state to states in the p_z- or d- like and higher states.
  - Predominantly z-polarization absorption. (QWIP-like; can activate with grating)
  - Also has weaker x,y-polarization (normal incidence) absorption.

Normal and 45° Incidence Response in Dot-in-the Well Structure



- 45° incidence yields stronger response
- Relative to the 45° response, the normal incidence response is much stronger than in QWIPs
- Similar behavior seen in QDIPs

Observation and Possible Explanations

- Relatively strong normal incidence response observed experimentally

- Simple effective mass model predicts no normal incidence oscillator strength for transitions from s-like ground state to p_z like states.

- Possible Explanations:
  - Band structure effects (due to mixing with other bands)
  - Impurity scattering Effects
    - Dopant hydrogenic wave function radius can be comparable to size of quantum dot
  - Transition to higher states

- Investigate theoretically

Theoretical Analysis

- Energy and wave functions computed using a stabilized transfer matrix technique by dividing the system into many slices along growth direction.
- Envelope function approximation with energy-dependent effective mass is used.
- Effective-mass Hamiltonian in k-sapce:

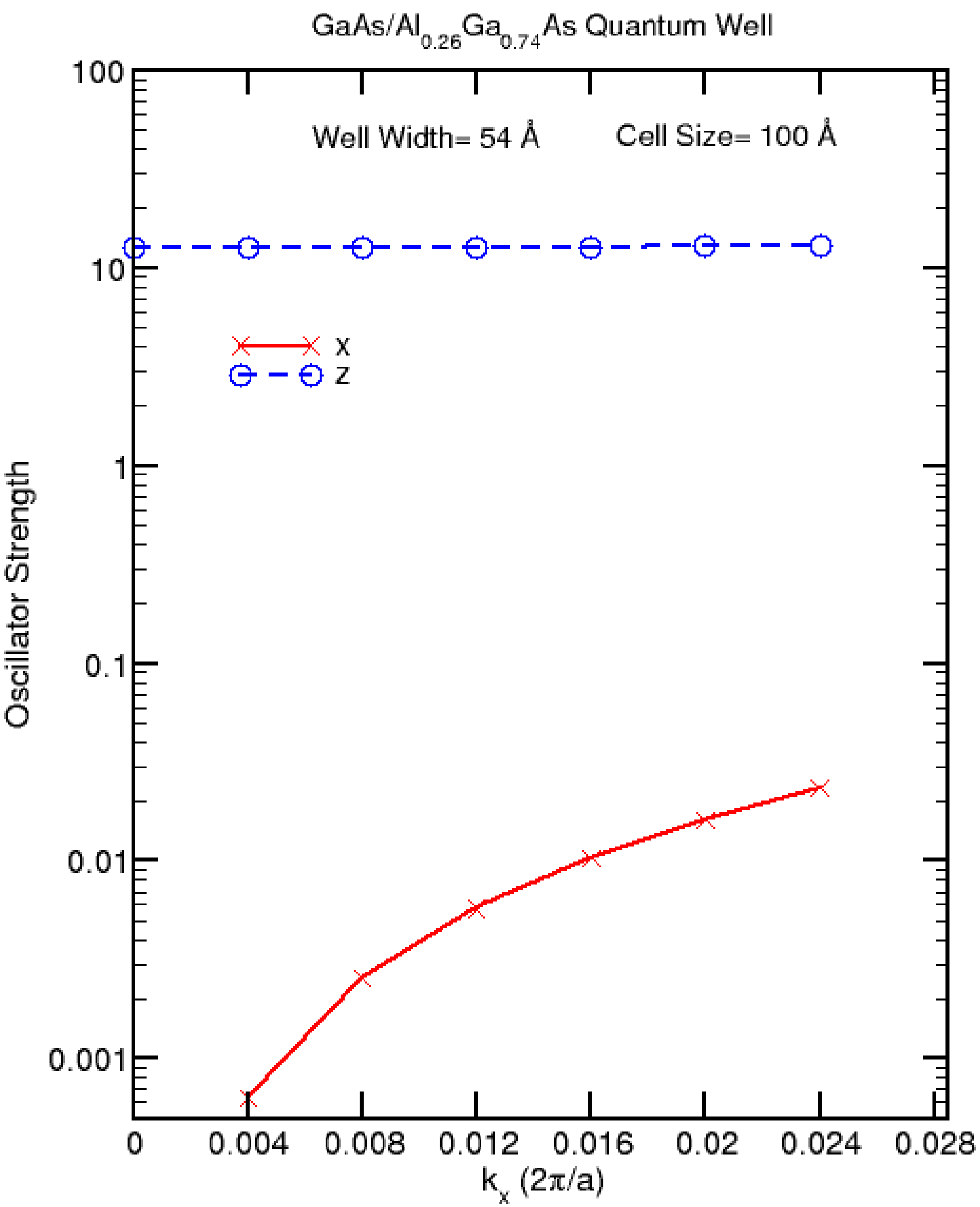
$$[(k_x^2+k_y^2)/m_t(E)+\partial_z^2/m_l(E)-E]F(\mathbf{k}) + \Sigma_{\mathbf{k}'}[V(\mathbf{k},\mathbf{k}')+V_{imp}(\mathbf{k},\mathbf{k}')]F(\mathbf{k}')=0$$

is solved via plane-wave expansion in each slice.

- 14-band k·p effects included perturbatively in optical matrix elements calculation
- Dopant effects incorporated as screened Coulomb potential
- The technique applies to quantum wells and quantum dots (or any 2D periodic nanostructures)

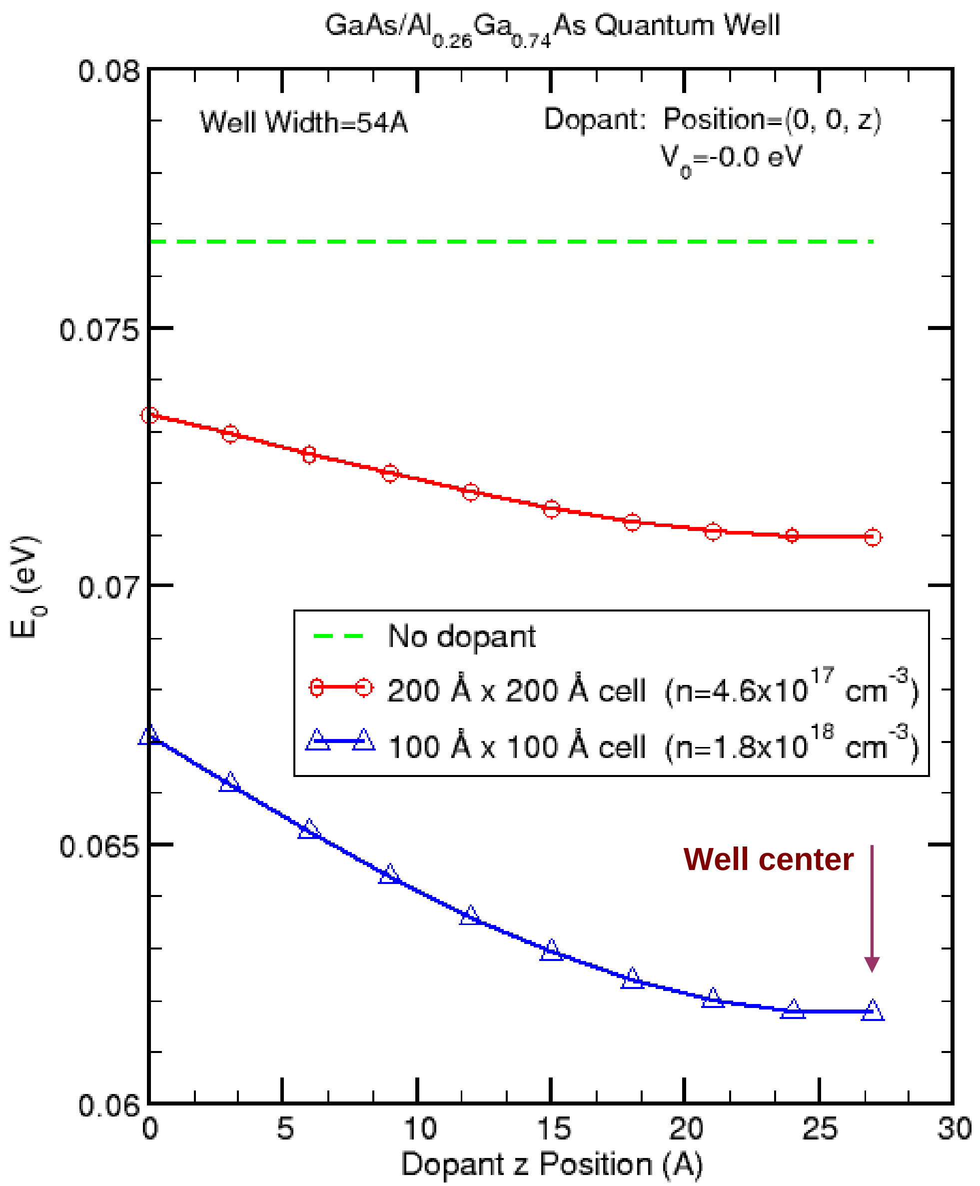
Quantum Well

Band Structure Effect on Oscillator Strengths



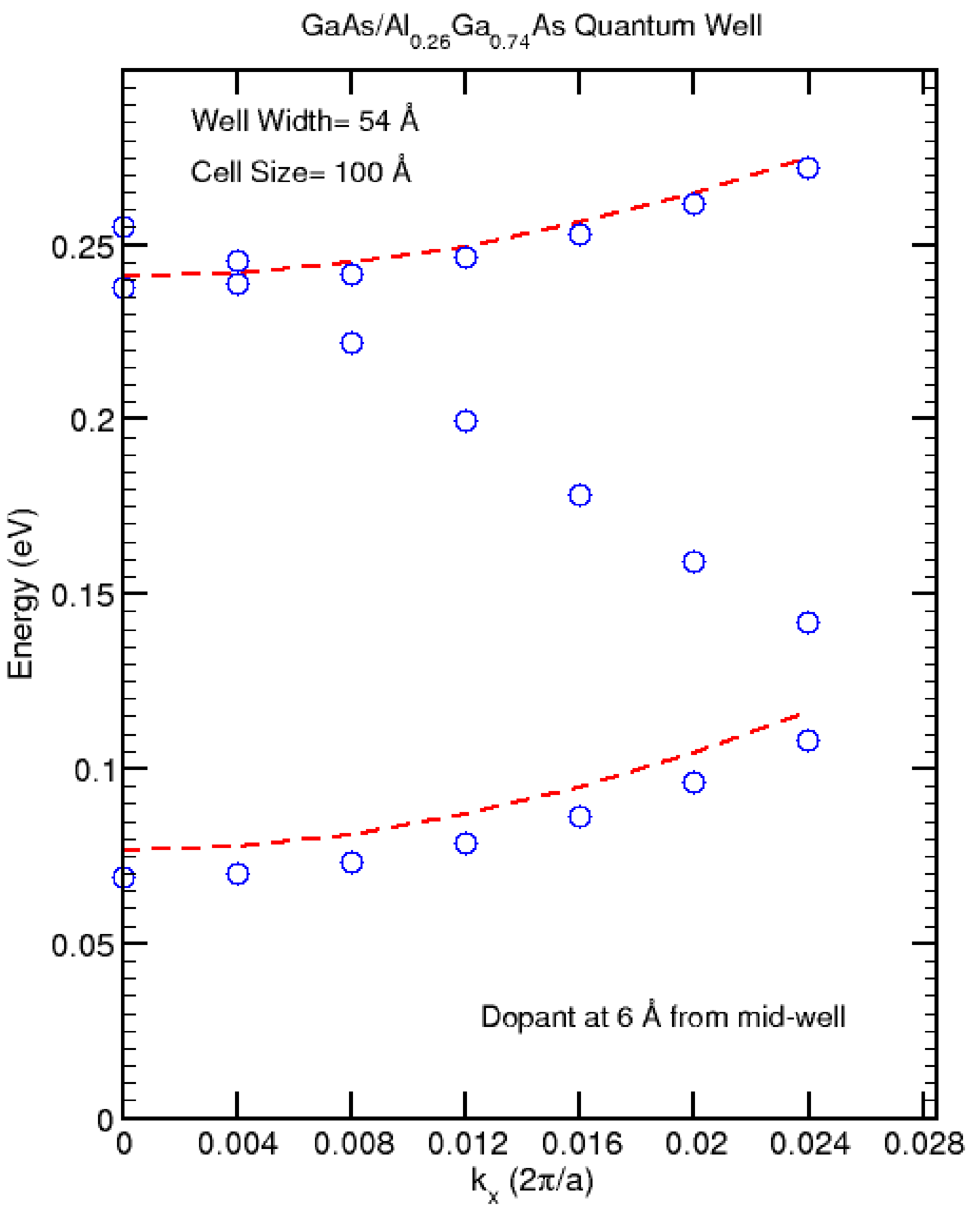
- $GaAs/Al_{0.26}Ga_{0.74}As$ quantum well
  - 54 Å wide GaAs well
- Band structure effect predicts > 0.2% x to z oscillator strengths ratio at k_x =0.02
- In general agreement with results reported in the literature

Ground State Energy with Impurity



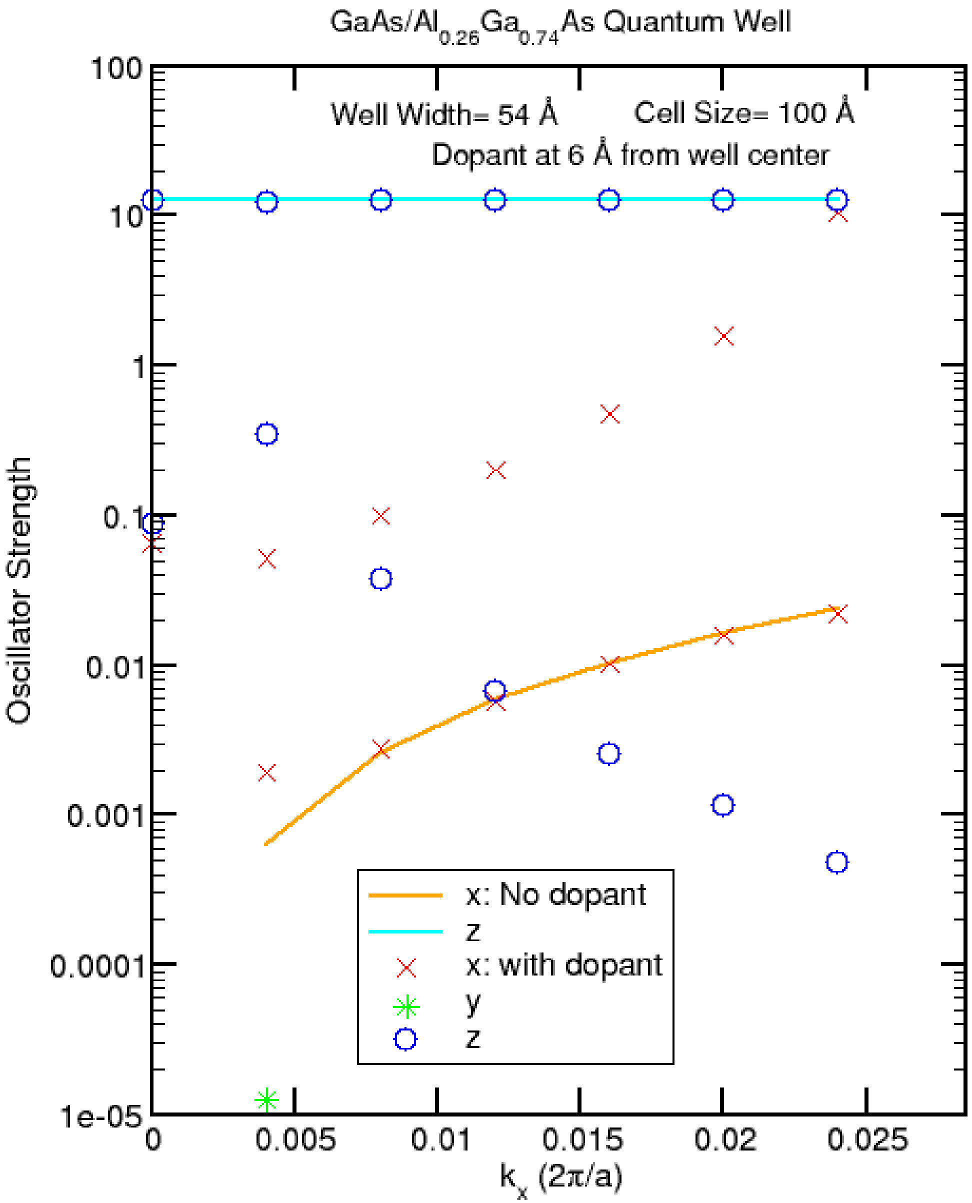
- With dopant, ground state energy vs. z-position (z=0 at edge, z=27 at well center)
- Green line is the ground state energy without dopants
- Single dopant simulation
- Different cell sizes used to simulate different doping concentration

Quantum Well Energy Levels with Dopant



- A single dopant is placed in a supercell with 100 Å lateral dimesnions
  - Dopant located at 6 Å from cell of the 54 Å wide GaAs well
- Dopant potential binding energy ~ few meV
- Supercell zone folding effects seen in energy levels

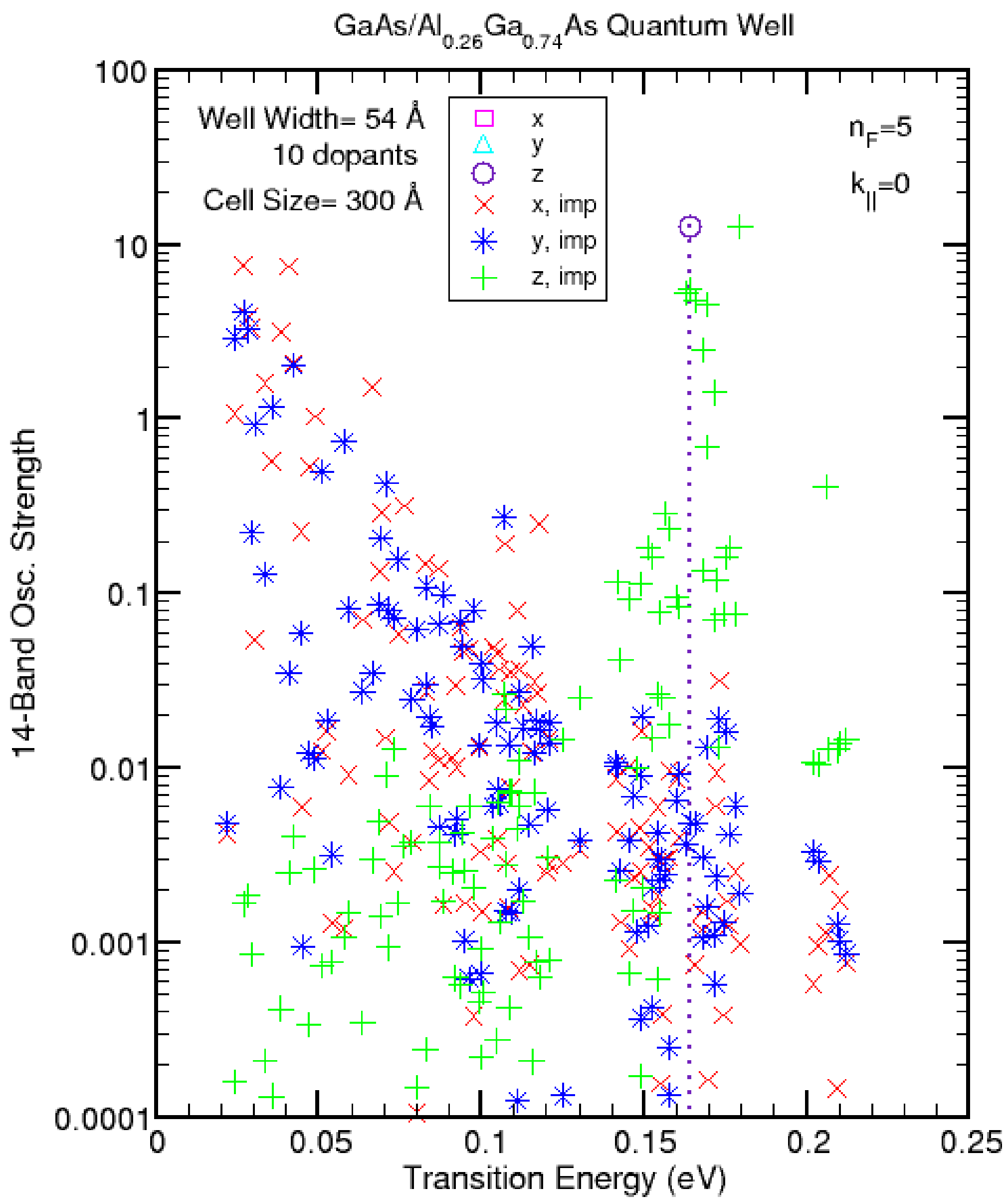
Dopant Effects on Oscillator Strengths



- Incorporation of dopant potential can increase the normal incidence oscillator strength

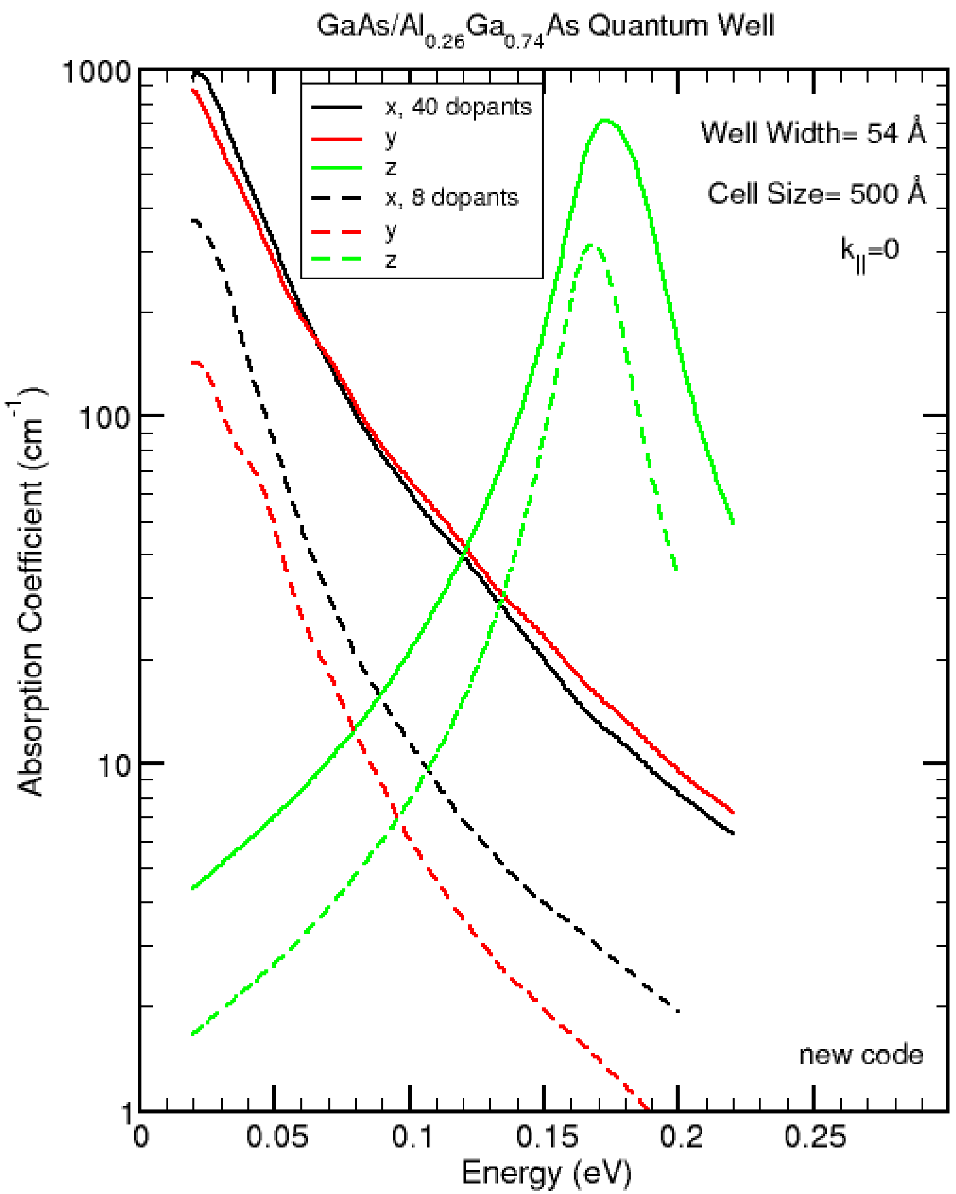
- More realistic simulations can be done using larger supercells with multiple randomly placed dopants

Dopant Effects on Oscillator Strengths



- Simulation geometry
  - Supercell with 300 Å lateral dimesnions
  - 10 randomly placed dopants in QW region of supercell
- Oscillator strength computed with the lowest 5 energy levels filled
- Only z oscillator strength when there is no dopant potential
- Dopants induce normal incidence oscillator strengths.

Absorption Coefficient



- 40 impurities and 8 impurities
- Low energy: intrasubband;
- xy dominant

Quantum Dot

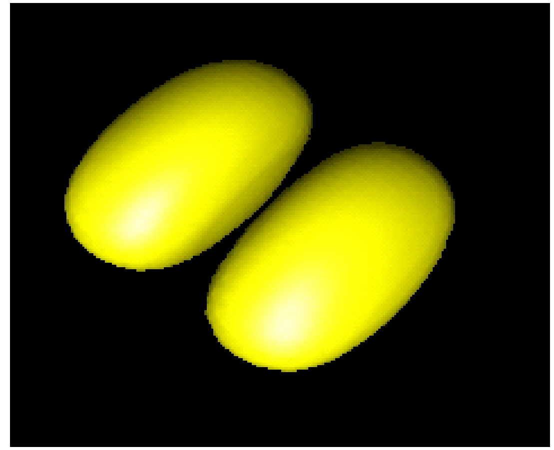
Simulation Geometry

<u>InAs quantum dot embedded in GaAs</u>

- Truncated pyramid (lens-shaped) QD on wetting layer
  - Base width 265 Å
  - Dot height 25 Å
  - Wetting layer thickness 5 Å
  - Lens shaped dot
- Incorporate dopant potential
  - Single dopant
  - Vary lateral position
  - Vary vertical position

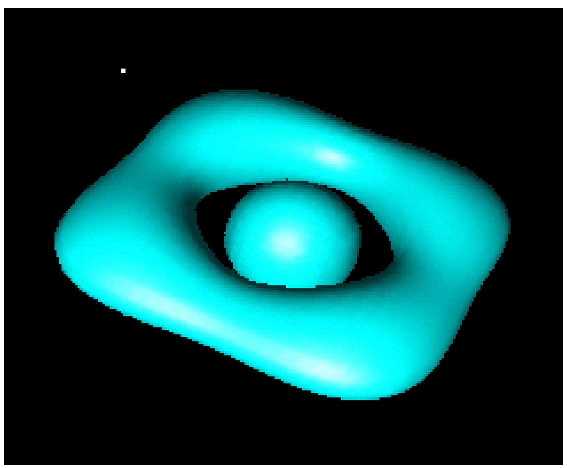
Charge densities of low-lying states in lens-shaped QD

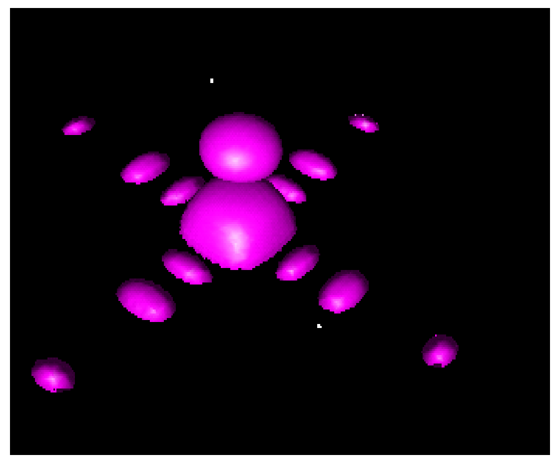
s-like



p_x/p_y like

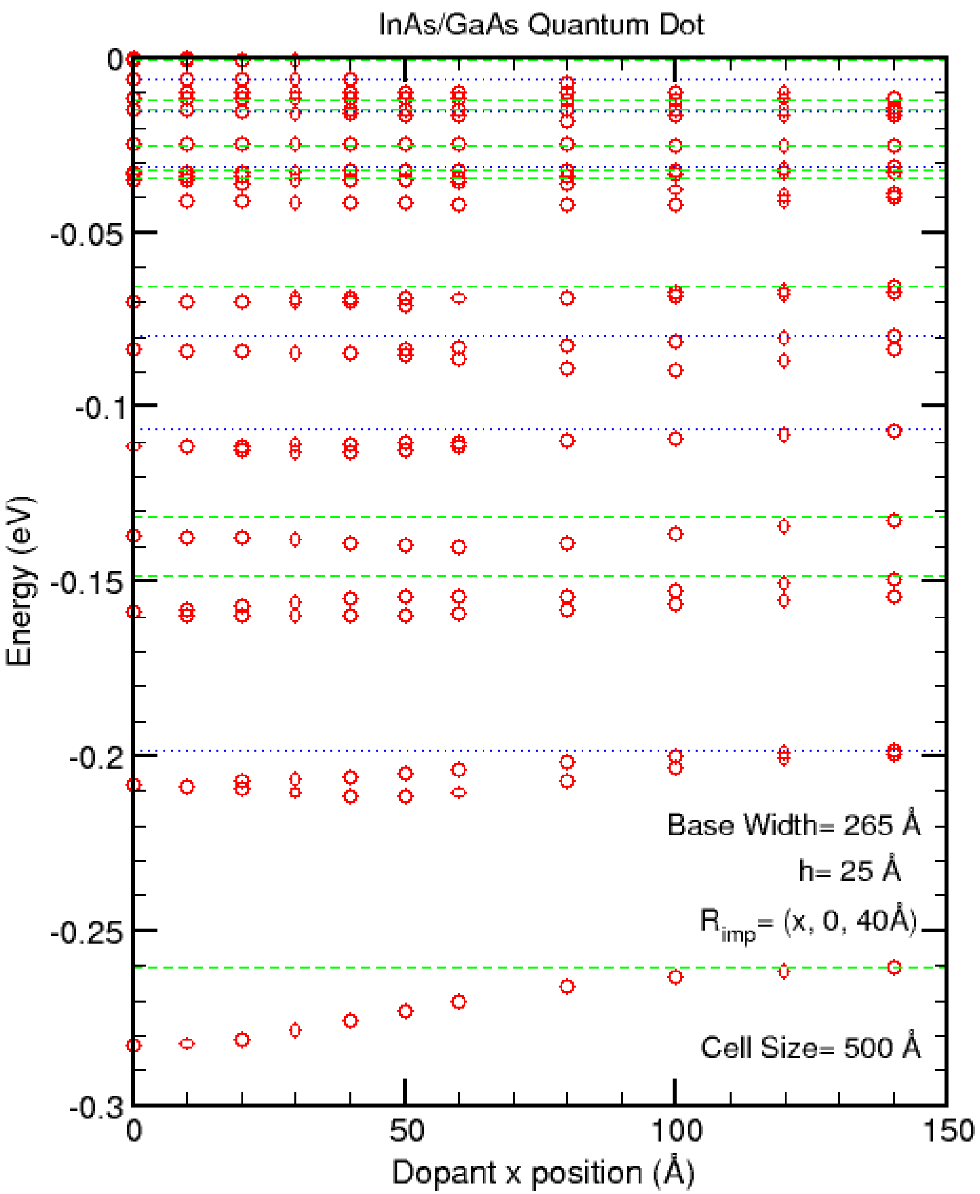
d-like





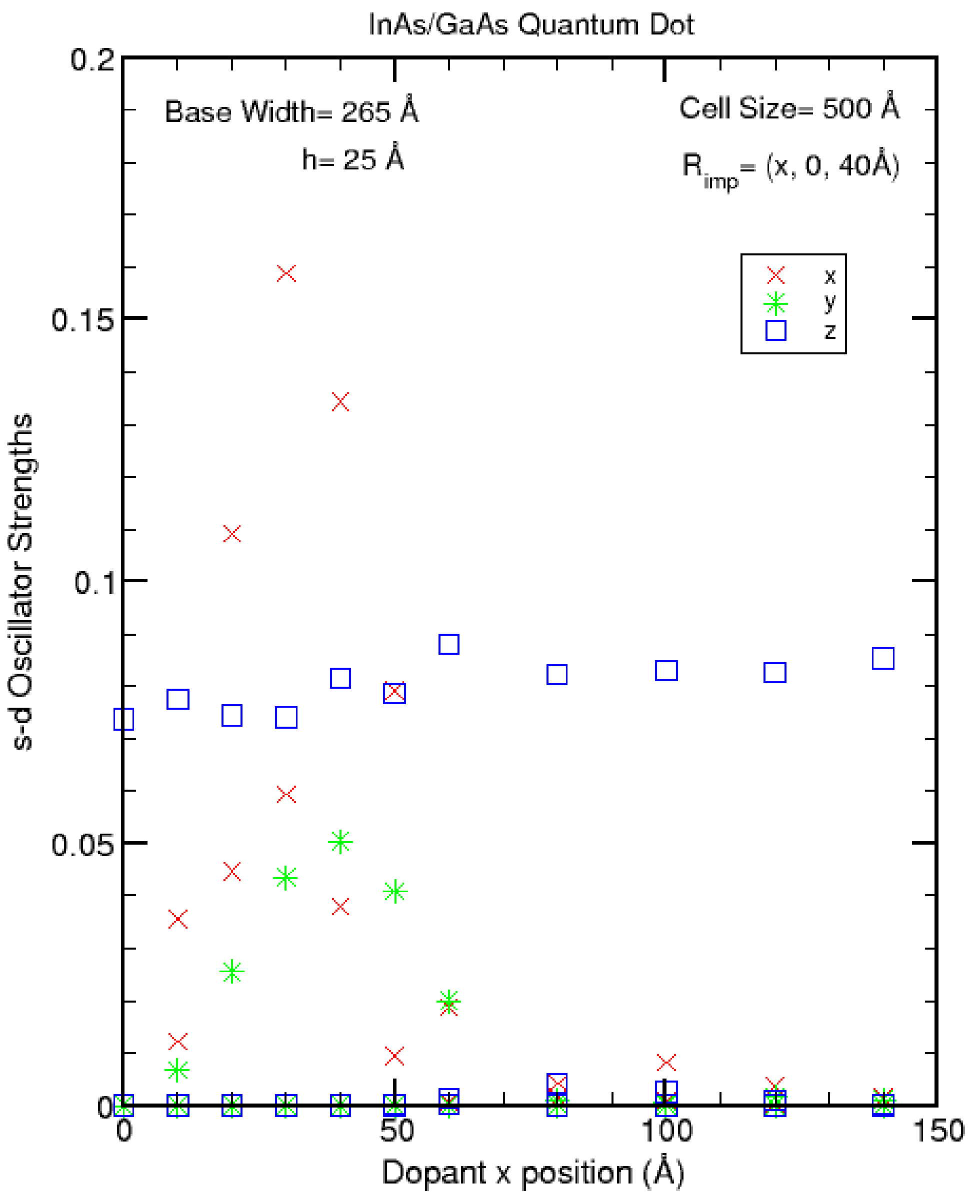
p_z like

Quantum Dot with Dopant Impurity Energy Levels



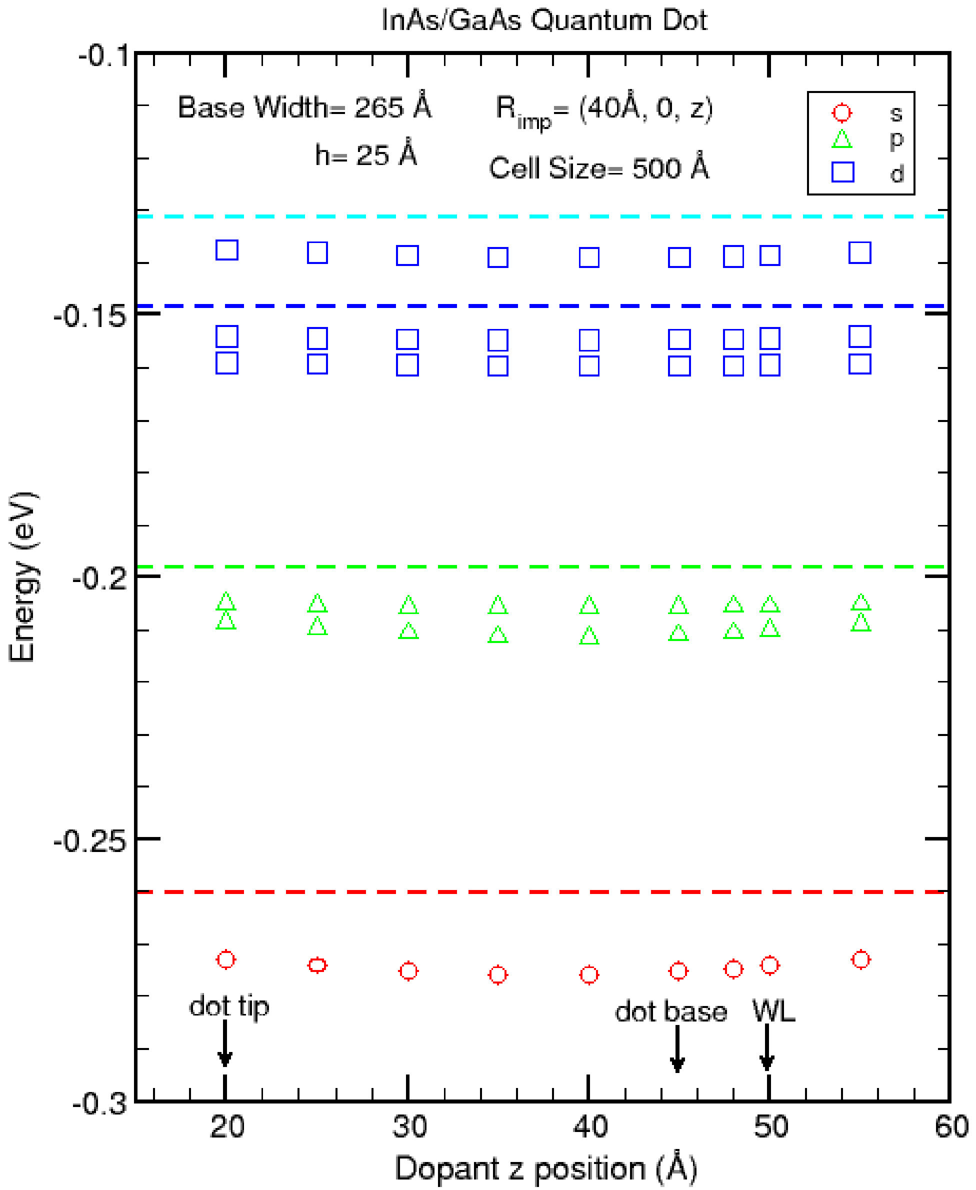
- Single dopant in a supercell
- Dopant position
  - Vary lateral (x) position
  - Vertical position fixed at 5 Å above top of wetting layer
- Energy level of QD with no dopant indicated by:
  - Green dashed line: even in x
  - Blue dotted line: odd in x
- Degeneracy removed by off center dopants

Effect of Dopant Potential on Oscillator Strengths



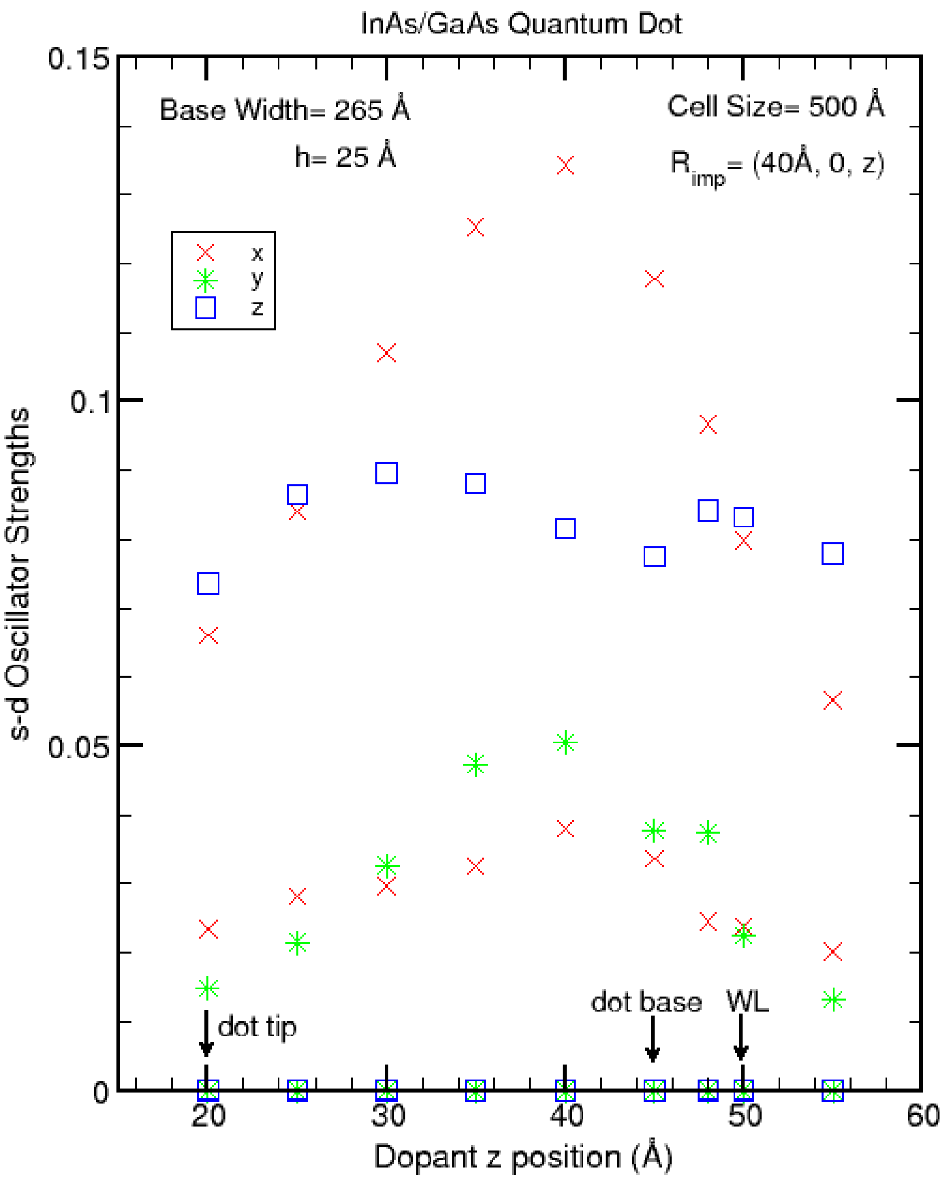
- Examine transitions from s-like ground state to 2nd set of excited states (d-manifold)
- No x oscillator strength without dopant potential
- With well-placed dopant, x oscillator strength can exceed z oscillator strength

Quantum Dot with Dopant Impurity Energy Levels



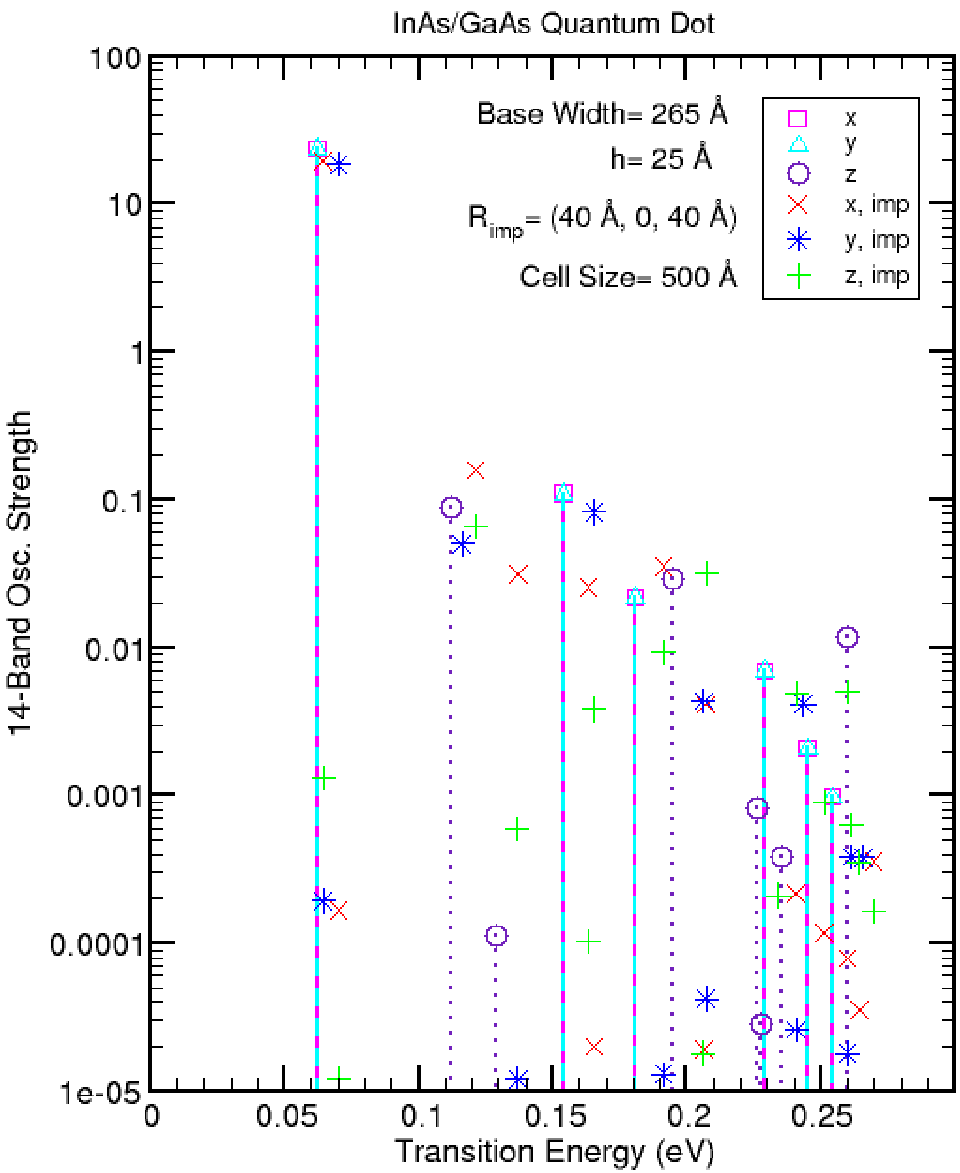
- Single dopant in a supercell
- Dopant position
  - Vary vertical (z) position
  - Lateral position fixed at 40 Å off center
- Energy level of QD with no dopant indicated by dashed lines
- Degeneracy removed by off center dopants

Effect of Dopant Potential on Oscillator Strengths



- Examine transitions from s-like ground state to 2nd set of excited states (d-manifold)
- Varying vertical position of dopant
- No x oscillator strength without dopant potential
- With well-placed dopant, x oscillator strength can exceed z oscillator strength

Effect of Dopant Potential on Oscillator Strengths



- Single dopant within the quantum dot
  - X: 40Å off center
  - Z: 5 Å above top of wetting layer
- No impurity oscillator strengths plotted as drop lines
  - X and y symmetric
- At transition energies above that of the fundamental (s-p) transition, dopant potential in general increases normal incidence oscillator strength at the expense of z oscillator strength

Summary

- Observed relatively strong normal incidence photoresponse in low-aspect ratio quantum dot devices
- Theoretical investigations indicate scattering due to dopant impurity potential could contribute to normal incidence response