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Investigation on the Photovoltaic Performance of Quantum Dot Solar Cells through Self-Consistent Modeling of Transport and Quantum Dot Carrier Dynamics

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Outline

- Motivation
- Physics-based model coupling transport and carrier dynamics
- Results
  - Model Validation: case study
  - Impact of QD e and h dynamics on $J_{sc}$ and $V_{oc}$
  - Modulation doped structures
- Conclusions
III-V Quantum Dots

- Attractive technology to enhance the efficiency of GaAs single- and multi-junction solar cells through bandgap and carrier dynamics engineering
- Possible method for the realization of Intermediate Band solar cells
- The actual potentiality is yet to be assessed
- Underlying physics involves a complex interplay between microscopic and nanoscopic processes → physics-based models are key to understanding the QD role on device performance

Typical device structure
State of art performance: undoped cells

- Small $J_{sc}$ increase, mainly due to WL photogeneration (from EQE measurements)
- $V_{oc}$ degradation
- Room Temperature performance dominated by thermal escape
State of art performance: doped cells

- **n-doping** (d-doping, direct doping) beneficial for $V_{oc}$ recovery
- some results have shown an increase of $J_{sc}$ with **n-doping**, whereas others do not show any significant improvement; **p-doping** kills $J_{sc}$
- The effect of **doping** is thought to modify the dynamics of capture and escape processes in/out the QDs ⇒ a model including **inter-sub-band carrier dynamics** may be useful to get deeper insight

**Sablons’s group**: Sablon et al. Nano Lett, 11, 2011

**Hubbards’s group**: to be published in IEEE JPV 2014
State-of-art modeling approaches

- Most models developed within the IB theory
  - Detailed balance principle, not suitable for device-level analysis
  - Device-level models based on drift diffusion complemented by a discrete energy level associated to the QD array ->
    - does not allow to describe inter-sub-band charge transfer between the QD states
    - suitable only for superlattice structures
This work: drift-diffusion + QD carrier dynamics *

- Tunneling escape from WL \( \rightarrow \) B can be included
- Considered only uncoupled QD layers

* M. Gioannini et al., IEEE JPV, 2013
Results

- Model Validation – Case study
  - Impact of QD e and h dynamics on $J_{sc}$ and $V_{oc}$
  - Modulation doped structures
Case study: correlation between QD size and photovoltaic performance

- $\Delta J_{sc}$ with respect to ref cell ~ integrated QD’s photogeneration rate: almost full collection efficiency
- Voc degradation larger for the larger QDs, i.e. with higher B-WL barrier
Results

- Model Validation – Case study

- Impact of QD e and h dynamics on $J_{sc}$ and $V_{oc}$

- Modulation doped structures
High collection efficiency despite slow electron dynamics $\rightarrow$ hole-driven dynamics!

$G_{ph}(WL)$

@ short circuit: high field $\rightarrow$ short sweep-out time in the Barrier

![Graph showing rates and time]
Escape/sweep-out “bottleneck” $\rightarrow V_{oc}$ degradation

- Under forward bias: lower electric field $\rightarrow$ higher barrier sweep-out time
- Capture/recombination becomes dominant over escape/sweep-out
- Effect as stronger as (higher) lower is the individual e/h (capture) escape
More on effect of e/h dynamics: “excitonic-like” case
QD contribution to $J_{sc}$ vs. e/h dynamics

hole dynamics much faster than electrons
→ linear (additive) behavior

“excitonic-like” case
→ NON linear behavior
QD contribution to $J_{sc}$ vs. e/h dynamics

"excitonic-like" case → NON linear behavior

Rates under full & filtered illumination

filtered ill., $\lambda > 870$ nm

full sun ill.
Results

- Model Validation – Case study
- Impact of QD e and h dynamics on $J_{sc}$ and $V_{oc}$
- Modulation doped structures
Modulation doping structures: $V_{oc}$ recovery in $n$-doped samples

- Dominant effect is suppressed electron capture from QDs
- Simulated $V_{oc}$ recovery $\sim 70$ mV for 8e/dot; p-doping quite ininfluent
- Experiments: 121 mV for 8e/dot $\delta$-doping (Polly et al., to appear in JPV 2014); 105 mV for 18e/dot direct doping (Lam et al., NanoEnergy 2014,)
Modulation doping structures: $J_{sc}$ and EQE
Conclusions

- Developed a device-level model including QD intersubband carrier dynamics and transport
- Simulated results in good agreement with typical experimental performance
- Highlighted impact of e/h individual dynamics and de-synchronization on apparent sub-bandgap collection efficiency and Voc degradation
- Preliminary analysis of modulation doped structures
Coupled drift-diffusion / QD model

\[
\frac{\partial E}{\partial x} = \frac{q}{\varepsilon} \left( p - n + N_d^+ - N_a^- + p_{WL} - n_{WL} + p_{ES_i} - n_{ES_i} + p_{GS_i} - n_{GS_i} \right)
\]

\[
\frac{\partial n}{\partial t} = \frac{\partial}{\partial x} \left( \mu_n n E + D_n \frac{\partial n}{\partial x} \right) - R_{TOT} + G_{PH} - R_{N_{CAP}} + R_{N_{ESC}}
\]

Photo-generation in the barrier

Capture from the barrier in the QDs

Photo-generation of carriers in the QDs

Escape of photo-generated carriers from the QDs to the barrier
QD Rate Equations

\[ \frac{\partial n_{WL_i}}{\partial t} = \frac{n_{WL_i}}{\tau_{nCAP}} - \frac{n_{WL_i}}{\tau_{nESC}} - \frac{n_{WL_i}}{\tau_{nCAP}} \left( 1 - \frac{n_{ES_i}}{N_D \mu_{ES}} \right) + \frac{n_{ES_i}}{\tau_{nESC}} + G_{PHWL} \]

\[ \frac{\partial n_{ES_i}}{\partial t} = \frac{n_{WL_i}}{\tau_{ES_i}} \left( 1 - \frac{n_{ES_i}}{N_D \mu_{ES}} \right) - \frac{n_{ES_i}}{\tau_{nESC}} - \frac{n_{ES_i}}{\tau_{nCAP}} \left( 1 - \frac{n_{GS_i}}{N_D \mu_{GS}} \right) + \frac{n_{GS_i}}{\tau_{nESC}} \left( 1 - \frac{n_{ES_i}}{N_D \mu_{ES}} \right) \]

\[ \frac{\partial n_{GS_i}}{\partial t} = \frac{n_{ES_i}}{\tau_{GS_i}} \left( 1 - \frac{n_{GS_i}}{N_D \mu_{GS}} \right) - \frac{n_{GS_i}}{\tau_{nESC}} \left( 1 - \frac{n_{ES_i}}{N_D \mu_{ES}} \right) \]

\[ G_{PHWL}(x, \lambda) = \int \alpha_{WL}(\lambda) \cdot \Phi_{AMI,SG}(\lambda) \cdot \exp \left(-\alpha_{WL}(\lambda) \cdot x \right) \cdot d\lambda \]

\[ G_{PHES}(x, \lambda) = \int \alpha_{ES}(\lambda, f_e, f_h) \cdot \Phi_{AMI,SG}(\lambda) \cdot \exp \left(-\alpha_{ES}(\lambda, f_e, f_h) \cdot x \right) \cdot d\lambda \]

\[ G_{PHGS}(x, \lambda) = \int \alpha_{GS}(\lambda, f_e, f_h) \cdot \Phi_{AMI,SG}(\lambda) \cdot \exp \left(-\alpha_{GS}(\lambda, f_e, f_h) \cdot x \right) \cdot d\lambda \]