NANOHOUR

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Beckman Institute - Room 3269

Computational studies of InAs/GaAs and InAs:Mn/GaAs quantum dot heterostructures for intermediate band solar cells

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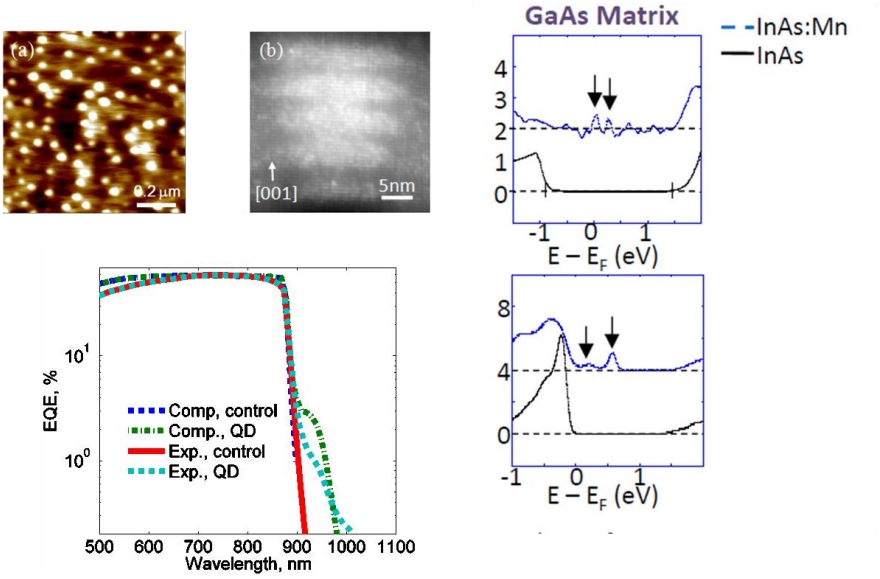
Semiconductor quantum dot (QD) heterostructures are widely used in photodetectors and have recently been proposed for use in highly-efficient intermediate-band solar cells (IBSC). In principle, absorption of photons via intermediate band transitions in these structures should generate additional photocurrent compared to absorption in more conventional *p-i-n* solar cells. Our recent calculations, along with results of experiments done by Professor Rachel Goldman's group at the University of Michigan, show that for a *p-i-n* solar cell containing InAs/GaAs quantum dots grown by MBE, transitions between the confined states in quantum dots do, indeed, allow some extension of the heterostructure absorption spectra beyond the GaAs absorption edge. In our calculations, we consider realistic QD morphological disorder, feeding the XSTM and AFM characterization results directly into our $\boldsymbol{k \cdot p}$ model. It was found that the heterostructure absorption spectra are highly sensitive to QD shapes and sizes. In order to more finely tune the IBSC electronic structure, the InAs quantum dots may be doped with manganese; in this case we compute the local electronic structure of Mn-doped quantum dots using moment-based order (N) tight binding. Our simulation results agree well with scanning tunneling spectra obtained by the Michigan group and show that additional in-gap states appear due to Mn doping on some of the In and Ga atoms. Our calculations explicitly account for the atomistic strain fields in the QD heterostructure through the use of Tersoff interatomic potentials and total energy minimization over the structure. Based on the experiments and calculations, the dopant atoms are most likely localized close to the edges of the InAs quantum dots, and the local density of states due to dopant atoms is highly sensitive to strain and composition. The results of this work will allow us to develop rules for the design of more highly efficient quantum dot based intermediate band solar cells.



Coffee and cookies will be served
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