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Enhanced confinement in compositionally heterogeneous alloy quantum dots ZUBAER HOSSAIN, University of Delaware — While there is a growing need to increase solar cell efficiencies and reduce the cost per watt, reported efficiencies are still well below the thermodynamic limit of photovoltaic energy conversion. The major factor that affects the efficiency (by more than 40%) is the lack of absorption or thermalization of electrons. To improve absorption, existing approaches, till date, are focused on combining multiple materials in the form of heterostructures. This talk will show the application of a physics-based mechanistic approach to engineer absorption by using alloy quantum dots and exploiting its heterogeneous compositional and deformation fields. Using a multiscale computational framework that combines density functional theory, k.p method and the finite element calculations, the work shows that heterogeneous distribution of composition and strain fields can lead to substantial confinement in alloy quantum dots. Subsequently alloy quantum dots that are much larger (on the order of 50 nm) in size – compared to their single crystalline counterparts (which are on the order of 5 nm) – can still provide significant confinement. The findings uncover new fundamental insights for engineering confinement that are unattainable under conventional homogenization approximations.

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