Abstract Submitted
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Mesoscale modeling of functional properties in core-shell nanoparticles[1] JOHN MANGERI, Department of Physics, University of Connecticut, Storrs, CT, United States, OLLE HEINONEN[2], Material Science Division, Argonne National Laboratory, Lemont, IL, United States, DMITRY KARPEEV, University of Chicago, Chicago, IL, United States, SERGE NAKHMANSON, Institute of Materials Science, University of Connecticut, Storrs, CT, United States
— Core-shell nanoparticle systems of Zn-ZnO and ZnO-TiO_2 are studied computationally using the highly scalable MOOSE finite-element framework, developed at Idaho National Lab. The elastic anisotropic mismatch of the core and shell create an imprinting effect within the shell that produces a wide variation of strains. Due to this diversity of strains, the sharp band gap edges of the bulk semiconductor are observed to be "thinned-out" much like amorphous silicon. We show that a variety of factors, such as particle size, core-to-shell volume ratio, applied hydrostatic pressure, shell microstructure, as well as the effect of surface elasticity, can influence the distribution of optical band-gap values within the particle, which may prove useful within the field of photovoltaics.

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