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Multiscale modeling of nanostructured ZnO based devices for optoelectronic applications: Dynamically-coupled structural fields, charge, and thermal transport processes.[1] ABDULMUIN ABDULLAH, SAAD ALQAHTANI, MD REZAUL KARIM NISHAT, SHAIKH AHMED, Southern Illinois University at Carbondale, SIU NANOELECTRONICS RESEARCH GROUP TEAM — Recently, hybrid ZnO nanostructures (such as ZnO deposited on ZnO-alloys, Si, GaN, polymer, conducting oxides, and organic compounds) have attracted much attention for their possible applications in optoelectronic devices (such as solar cells, light emitting and laser diodes), as well as in spintronics (such as spin-based memory, and logic). However, efficiency and performance of these hybrid ZnO devices strongly depend on an intricate interplay of complex, nonlinear, highly stochastic and dynamically-coupled structural fields, charge, and thermal transport processes at different length and time scales, which have not yet been fully assessed experimentally. In this work, we study the effects of these coupled processes on the electronic and optical emission properties in nanostructured ZnO devices. The multiscale computational framework employs the atomistic valence force-field molecular mechanics, models for linear and non-linear polarization, the 8-band sp^3s^* tight-binding models, and coupling to a TCAD toolkit to determine the terminal properties of the device. A series of numerical experiments are performed (by varying different nanoscale parameters such as size, geometry, crystal cut, composition, and electrostatics) that mainly aim to improve the efficiency of these devices.

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