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elasticity model and the valence force field method (VFF) by projecting the deformation polarization-field [12] onto the atomic positions. The VFF method improves the quality of the local relaxation calculation around the In ions and corrects for internal strain effects. The validity of this coupled approach for small linear deformations has been discussed in [13]. In order to couple the atomistic calculation of electronic states with the continuous media model for particle transport, the macroscopic electrostatic potential calculated with the Poisson/drift-diffusion model is projected onto the atomic positions. The solution of the eigenvalue problem resulting from ETB provides the spatial probability density (SPD) and the probabilities of optical transitions. The used ETB model is based on a reliable sp3d5s* parametrization [14]. In the case of ETB, the resulting density was projected onto the finite element mesh used for the continuous media models. This projection is done using an exponentially decaying function centered on each atomic site. **3 Results** Our LED model shown in Fig. 1 use an intrinsic 3nm-thick InGa_N QW for the active region and 3nm Ga_N material for lateral barriers. The n-side is 45.5 nm and the p-side is 42 nm. A 2.5-thick nm cell for the QW has been considered for periodicity along Y and Z axes which defines the geometry to the atomistic builder in order to construct a 3D model (top figure). 2016 Several studies reported that organic solar cells offer good power conversion efficiency (PCE) [8]–[12] through modification of material properties such as energy levels and charge collection at electrode by interface engineering and optimization of the morphology of the active film [13]–[16]. The main limitations of OPVs are related to the limited absorption spectrum [17]–[18] and low carrier mobility of organic semiconductors, in the range of 10⁻⁵–10⁻¹ cm²/V·s [19]–[21]. Whereas generally in solar cells, the mobility can be controlled only to a limited extent, the absorption efficiency can be improved considerably by connecting two or more cells absorbing in different spectral ranges in the tandem configuration. By stacking several subcells in series configuration, theoretical limits for an ideal

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