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Continuum and KMC simulations of realistic bulk heterostructure solar cell photovoltaic devices KANOKKORN PIMCHAROEN, DANIEL OLDS, PHILLIP DUXBURY — Design of novel solar cell architectures is significantly assisted by reliable continuum device models, and computational methods capable of solving these models in one, two and three dimensions. We are developing computational methods for these models and are validating them using Kinetic Monte Carlo simulations in the same morphologies. We present simulations using idealized morphologies to test approximations in the continuum models, and we present results for bulk heterostructure morphologies deduced by refining digital nanostructures to experimental neutron relectometry and small angle scattering data. In particular we discuss the ability of one dimensional device models to capture the physics of photovoltaic response of realistic bulk heterostructures.

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