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Master Equation Approach to the Simulation of Transport Properties in Materials with Structural and Site-Energy Disorder AVADH SAXENA, Los Alamos National Lab, IVO BATISTIC, University of Zagreb, Croatia, ENRIQUE BATISTA, RICHARD MARTIN, DARRYL SMITH , Los Alamos National Lab — The study of diorder in crystalline materials assumes an underlying lattice. However, many materials such as conducting polymers and amorphous semiconductors do not in general have an underlying lattice. Therefore, instead of a lattice a network with disorder must be considered. To this end, we apply the master equation approach to a network in order to study transport properties of materials that exhibit both structural and site-energy disorder. The level of disorder is characterized by several parameters such as energy distribution function, spatial correlation function, fluctuations in the number of nearest neighbors or distance between them. We calculate mobility as a function of temperature and applied electric field for different levels of the disorder. The theory is also applicable to other materials such as organic semiconductors.

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