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A model of dopant diffusion through a strongly correlated p-n junction. JEDRZEJ WIETESKA, Columbia University, RICHARD BRIERLEY, Yale University, GIAN GUZMAN-VERRI, University of Costa Rica and Argonne National Laboratory, GUNNAR MOLLER, University of Cambridge, PETER LITTLEWOOD, Argonne National Laboratory, University of Chicago, LITTLEWOOD GROUP COLLABORATION — The diffusion of charged ions in a solid depends on an equation of state that balances diffusive and screened electrostatic forces, and is well understood in the case of conventional semiconductors and metals. In the case of a strongly-correlated material, the physics is different, and expected to be relevant, for example, in Li-ion battery cathodes. We propose a model of dopant ion motion through a strongly correlated p-n junction. Our approach is to consider diffusive (Nernst-Planck) dynamics of dopants under screened electrostatic interactions computed [1] within a mean-field (Thomas-Fermi) approximation. Dopant profiles as function of time are calculated for a p-n junction held at constant voltage. In the case where filling levels are near a correlation-induced gap, Mott insulating regions can form at the p-n interface and their dynamics is studied. References: 1. Charlebois et al., Phys. Rev. B, 87 035137 (2013)

Jedrzej Wieteska
Columbia University

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