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From Light Impurity Doping to Complete Cation Exchange in Semiconductor Nanocrystals: The Role of Coulomb Interactions STEVEN ERWIN, Naval Research Lab, FLORIAN OTT, DAVID NORRIS, ETH Zurich —
Cation exchange is a reversible chemical reaction used to create new materials by replacing one type of cation with another, usually from solution. We have developed an atomistic model describing cation exchange in semiconductor nanocrystals. The model uses a small set of results obtained from DFT calculations for Ag-doped CdSe. From these we constructed a kinetic Monte Carlo model to address finite temperatures and time scales beyond the reach of DFT. Our simulations span a wide range of Ag concentrations, from light doping to full cation exchange. Thus our model provides a single conceptual framework in which these two phenomena can be understood as limiting endpoints. The results of the simulations are consistent with several experimentally observed aspects of both phenomena. An unexpected finding of our simulations is that the Coulomb interaction plays a central, but changing, role as the Ag concentration varies from light doping to fully cation exchanged. For example, if the Coulomb interaction is strongly screened then cation exchange is suppressed or stopped. When only moderately screened, Coulomb effects play an unanticipated but important role for both doping and cation exchange.

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