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Self-purification in semiconductor nanostructures[1] GUSTAVO DALPIAN, Universidade Federal do ABC, JAMES R. CHELIKOWSKY, University of Texas — Doping semiconductors is an important process in order to develop functional devices with them. This suggests that, when dealing with semiconductor nanostructures, they should also be doped in order to broaden their possible applications. Experimentally this shows to be a very difficult task. "Self-purification" mechanisms are often claimed to make this task even more difficult, as the distance a defect or impurity must move to reach the surface of a nanocrystal is very small. Kinetic effects like this are usually invoked in order to explain this difficulty. Here we show that self-purification can be explained through energetic arguments and is an intrinsic property of defects in semiconductor nanocrystals. We find the formation energies of defects increases as the size of the nanocrystal decreases. This is due to the pinning of the impurity levels as the size of the nanocrystal decreases and experimental evidences support our argumentation. We analyze the case of Mn-doped CdSe nanocrystals and compare our results to experimental findings, proposing ways to improve their dopability.

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