

Abstract Submitted
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Efficient n -type doping of zinc-blende III-V semiconductor quantum dots¹ LUCAS V. BESTEIRO, LUIS TORTAJADA, Universidad de Santiago de Compostela, Spain, MURILO L. TIAGO, University of Texas at Austin, L.J. GALLEGO, Universidad de Santiago de Compostela, Spain, JAMES R. CHELIKOWSKY, University of Texas at Austin, M.M.G. ALEMANY, Universidad de Santiago de Compostela, Spain — Semiconductors are intentionally doped n -type by replacing one host atom by an impurity atom that has one more electron. In the case of III-V semiconductors this can be done at both anion and cation sites. Here we show that III-V semiconductor nanocrystals with zinc-blende structure should not be doped by cation substitution, but rather by anion substitution. We found that, as result of quantum confinement, the formation of defects that affect the main characteristics of the dopants is favored when the nanocrystals are doped at the cation site. Our study is performed through first-principles calculations based on a real-space implementation of density-functional theory and pseudopotentials by using the PARSEC code.

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