

Abstract Submitted
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Efficient n -type doping of zinc-blende III-V semiconductor nanowires¹ LUCAS V. BESTEIRO, LUIS TORTAJADA, J. SOUTO, L.J. GALLEGO, Universidad de Santiago de Compostela, Spain, JAMES R. CHELIKOWSKY, The University of Texas at Austin, M.M.G. ALEMANY, Universidad de Santiago de Compostela, Spain — We demonstrate that it is preferable to dope III-V semiconductor nanowires by n -type anion substitution as opposed to cation substitution. Specifically, we show the dopability of zinc-blende nanowires is more efficient when the dopants are placed at the anion site as quantified by formation energies and the stabilization of DX -like defect centers. The comparison with previous work on n -type III-V semiconductor nanocrystals also allows to determine the role of dimensionality and quantum confinement on doping characteristics of materials. Our results are based on first-principles calculations of InP nanowires by using the PARSEC code.

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