Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

The role of quantum confinement in p-type semiconductor InP nanocrystals[1] LUIS TORTAJADA, M.M.G. ALEMANY, 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 — We characterize the impurity state responsible for current flow in Zn-doped InP nanocrystals through first-principles calculations based on a real-space implementation of density-functional theory and pseudopotentials. We found the activation energy of the acceptor state to range from 0.03 eV in the bulk to 2.5 eV in smaller nanocrystals as a result of quantum confinement. The maximum value for nanocrystals is an order of magnitude larger than the maximum value found for InP nanowires (0.2 eV). Our results show that reducing the dimensionality in p-type InP materials strongly inhibits the capability of the materials to generate free carriers.

[1]Work supported by the Xunta de Galicia (Educacion e Ordenacion/FEDER, INCITE08PXIB206107PR and INCITE08E1R206041ES), MICINN/FEDER (FIS2008-04894/FIS and Program Ramon y Cajal), and the DoE (DE-FG02-06ER46286). Computational support provided by CESGA.

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Date submitted: 17 Dec 2009 Electronic form version 1.4