Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

***Ab initio* calculations for the electronic properties of zinc-doped indium phosphide nanowires**[1] MANUEL ALEMANY, Universidad de Santiago de Compostela, Spain, XIANGYANG HUANG, University of Minnesota, 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 — p-type indium phosphide nanowires are known to function as working devices when assembled with n-type nanowires, and thus are seen as very promising building blocks for highly integrated electronic devices within the semiconductor industry. In this work, we have characterized the impurity state responsible for current flow in zinc-doped indium phosphide nanowires through first-principles calculations based on a real-space implementation of density-functional theory and pseudopotentials. The binding energy of the acceptor state is predicted to range from the value of the acceptor state in the bulk to up to values of approximately 0.2 eV in the thinner nanowires as a result of the two-dimensional quantum confinement. Our results show that, in thin nanowires, quantum confinement can move the defect level deep into the energy gap.

[1]Work supported by the Spanish Ministry of Education and Science (Program "Ramon y Cajal" and Project FIS2005-04239), by the NSF, by the DOD, by the Barcelona Supercomputing Center, by the Galician Supercomputing Center, and by TACC.

Manuel Alemany
Universidad de Santiago de Compostela, Spain

Date submitted: 26 Nov 2007 Electronic form version 1.4