

Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

First principles investigation of InN non-polar surfaces and nanowires¹ ALEKSANDRS TERENTJEVS, Politecnico of Torino, Torino, Italy, ALESSANDRA CATELLANI, CNR-IMEM, Parma, Italy, GIANCARLO CICERO, Politecnico of Torino, Torino, Italy — In the last years InN nanostructures have been proposed for application in solar cells, because of the outstanding electronic properties of this nitride compound. An increase of solar energy conversion in these kinds of cells requires a deep knowledge of surfaces properties, and on the effect of confinement on the electronic properties of the material. Here we present an investigation of the structural and electronic properties of InN nanowires as obtained by means of *ab initio* Density Functional calculations. First we discuss the results for the clean (1-100) and (11-20) faces, which are usually exposed in nanostructures, then we show how InN electronic properties change in nanowires due to confinement effects. We will finally present a possible InN functionalization pathway based on the use of molecules containing thiol groups. Our results show that thiols may attach to the surface following an exothermic process (dissociation energy is about 2.5 eV/mol for the (11-20) surface), thus they represent an effective anchoring group for the realization of hybrid InN based devices.

¹This work was supported, within the EU FP6, by the ERANET project “NanoSci-ERA: NanoScience in the European Research Area”

Giancarlo Cicero
Politecnico of Torino, Torino, Italy

Date submitted: 02 Dec 2007

Electronic form version 1.4