Abstract Submitted for the MAR10 Meeting of The American Physical Society

Theoretical investigation of the InN/In2O3 interface GIANCARLO CICERO, ANTONIO ALIANO, Materials Science and Chemical Eng. Dep., Politecnico of Torino, Italy, ALESSANDRA CATELLANI, CNR-IMEM, Parma, Italy, NANOLICHT COLLABORATION — Indium Nitrides (InN) nanowires (NWs) have attracted lot of attention because of their potential applications in optoelectronics and solar cells. Recent XPS measurements on collections of InN NWs showed that a thin amorphous oxide layer (In2O3) at the InN NW surface is formed upon exposure to air, altering the electronic properties of the NWs [1]. A deep understanding of the electronic properties of amorphous In2O3 and of the InN/In2O3 interface assume great relevance in the clarification on the NWs electronic properties and it can shed light on the surface contribution to their conductivity. Motivated by this experimental evidence, we have undertaken a combined classical and ab initio theoretical investigation of amorphous In2O3 and of a realistic In2O3/InN interface. Here we discuss the properties of these systems evidencing the difference and similarities between the In2O3 amorphous and crystalline structure first and than presenting how the level alignment at the In3O3/InN heterostructure may affect InN NWs features. [1] F. Werner et al., Nano Letters 9, 1567 (2009)

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