



ΓΕΝΙΚΟ ΣΕΜΙΝΑΡΙΟ ΤΜΗΜΑΤΟΣ ΦΥΣΙΚΗΣ

PHYSICS COLLOQUIUM

Thursday, 19 December 2013

17:00 -18:00

3rd Floor Seminar Room

**“Limits of In incorporation on $\text{In}_{1-x}\text{Ga}_x\text{N}$ {0001} surfaces:
an ab initio approach”**

Dr. Liverios Lymperakis

Max-Planck Institut für Eisenforschung GmbH

Abstract

There is great interest in using InGaN as the active layer in optoelectronic devices: Owing to a tunable direct bandgap ranging from 0.7 eV for InN to 3.4 eV for GaN almost the entire spectral range can be accessed by varying the In concentration. However, the growth of high quality, In-rich InGaN films is affected by In surface segregation, low growth temperatures, spinodal decomposition and phase separation. In this work we investigate the thermodynamics of In incorporation into the technologically relevant (0001) (Ga-polar) and (000-1) (N-polar) surfaces using density functional theory. The cases of coherent pseudomorphic growth on GaN and on lattice-matched heterointerfaces are considered. Our results show that, in agreement with previous experiments, larger In incorporation in N-polar than Ga-polar surfaces can be achieved for the same growth conditions. Based on our calculations we derive an on-atomic-scale understanding of In incorporation in InGaN surfaces and the physics underlying the aforementioned finding we be discussed.