UNIVERSITY OF CRETE
DEPARTMENT OF PHYSICS

CRETE CENTER FOR
QUANTUM COMPLEXITY
AND NANOTECHNOLOGY

ΓΕΝΙΚΟ ΣΕΜΙΝΑΡΙΟ ΤΜΗΜΑΤΟΣ ΦΥΣΙΚΗΣ

PHYSICS COLLOQUIUM

Thursday, 05 March 2015

17:00 -18:00

3rd Floor Seminar Room

"Insights in III-Nitride surface thermodynamics, kinetics and electronic structures from first principles"

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Abstract

Understanding the thermodynamics, kinetics, and electronic structure of surfaces is of particular interest for epitaxially grown semiconductors: The surface morphologies and quality of the film as well as the optoelectronic properties (e.g. surface Fermi level, free carrier concentration, and conductivity) depend sensitively on these. Ab initio calculations constitute a well established tool which can be applied in understanding, explaining, and /or guiding experiment and can provide information which is not directly/straightforwardly accessible by the latter. In this talk ab initio based investigations on the technologically relevant III Nitride surfaces will be presented. In the first part the atomistic mechanisms underlying the antisurfactant effect of Si in the growth of GaN will be addressed. In the next part the electronic structure of polar and non-polar GaN surfaces as well as the interplay between thermodynamics and kinetics of H2 adsorption on them will be presented. Based on the aforementioned calculations the effect of surfaces on the growth and the optoelectronic properties of the material will be discussed. Furthermore, the aforementioned topics will be used as examples to demonstrate and highlight the ability of first principles calculations in explaining growth, HRTEM, x-ray and ultraviolet photoelectron spectroscopy and in guiding and designing STM experiments.