ΣΕΜΙΝΑΡΙΟ ΚΕΝΤΡΟΥ ΚΒΑΝΤΙΚΗΣ ΠΟΛΥΠΛΟΚΟΤΗΤΑΣ & ΝΑΝΟΤΕΧΝΟΛΟΓΙΑΣ/ CCQCN SEMINAR

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15:00-16:00

3rd Floor Seminar Room

Epitaxial Grown of III-Nitrides: Insights from Density Functional Theory Calculations

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Abstract

GaN and related group III-Nitrides are materials of choice for high temperature and high power microelectronic devices as well as for solid state lighting. However, in molecular beam epitaxy (MBE), the use of low pressures, the high melting temperatures of GaN, and the extremely large binding energy of the N_2 molecule make the growth of high quality films with smooth surface morphologies challenging. Furthermore, the growth of high In content $In_xGa_{1-x}N$ alloys, as required e.g. to achieve green emission, is challenging due to a complex competition between strain and chemistry arising from the different Indium and Gallium atomic radii as well as their different bonding enthalpies with nitrogen. The aforementioned mechanisms constitute the driving force towards phase separation through spinodal decomposition. A first step towards achieving full control on the growth and the properties of III-Nitride alloys is to gather a fundamental understanding of the thermodynamics and kinetics underlying the growth of these materials. In the present talk we will demonstrate how density functional theory (DFT) calculations can be used to address the surface and bulk thermodynamics and kinetics and to provide insights on the atomic scale mechanisms and the physics governing the growth and the properties of these alloys. In the first part of the talk the DFT methodology will be briefly discussed. Next, based on earlier as well as recent works, we will discuss how the aforementioned methodology can be applied to explain and guide growth and characterization experiments and address the above mentioned challenges. The dependence of surface morphologies and reconstructions on the growth conditions, the Indium incorporation and surface segregation as well as the bulk thermodynamics of the $In_{1-x}Ga_xN$ alloys will be used as case studies. Based on these results we will derive and discuss the peculiarities and the general trends and physics underlying the growth of the technologically important III-Nitride materials.