

# 9<sup>th</sup> International Conference on Nanosciences & Nanotechnologies (NN12)

3 - 6 July 2012, I.Vellidis Congress Center  
Thessaloniki, Greece

# ABSTRACT BOOK

## PLENARY SPEAKERS (common with ISFOE12)

Phaedon Avouris, IBM, USA  
Alex Zunger, Univ. Colorado, USA  
George Malliaras, EMSE, France

## KEYNOTE SPEAKERS

Norbert Koch, Humboldt-Universität zu Berlin, Germany  
George Hadziioannou, LCPO, CNRS, France  
S. Ravi P. Silva, Univ. of Surrey, UK  
Takeshi Akasaka, TARA Center, Univ. of Tsukuba, Japan  
Luis Echegoyen, Univ. of Texas at El Paso, USA  
Ioannis Missirlis, Univ. of Patras, Greece  
Thimios Mitsiadis, Univ. of Zurich, Switzerland  
Konstantin Gus Kousoulas, Louisiana State Uni, USA  
Hans Jorg Meisel, BG-Clinic Bergmannstrost, Germany  
Efthimios Kaxiras, Harvard Univ., USA  
Rena Bizios, Univ. of Texas at San Antonio, USA

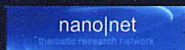
## NANOTECHNOLOGY 2012

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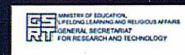
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## Laser annealing and simulation of a:Si thin films for solar cell applications

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I. Raptis<sup>1</sup>, D. Tsoukalas<sup>1</sup>, I. Zergioti<sup>1</sup>

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In this work we are demonstrating the implementation of Nd:YAG laser annealing for the partial crystallization of an amorphous silicon layer, in order to improve its solar cell efficiency. A Nd:YAG laser (FWHM=6 ns, energy ranging from 25 to 80 mJ) with air as an ambient medium has been used at two different wavelengths (532 and 1064 nm), in order to determine the optimum annealing conditions for the realization of the partial crystallization of a-Si layer. The laser experimental work is combined with simulation of the annealing effect, in terms of temperature distribution evolution, using the Synopsys Sentaurus Process TCAD software, so as to predetermine the optimum annealing conditions at each laser wavelength. In both cases irradiations took place in the sub-melt regime, so as to avoid significant diffusion occurrence on the p and n doped layers within the structure. Annealed samples are subsequently characterized by means of SEM, XRD and RAMAN in order to investigate the effect of the irradiation on the crystallization of a part of a-Si layer, at the desired depth.

## Modelling of excited-state properties of novel phosphorescent iridium complexes

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Organic light-emitting diodes (OLEDs) are one of the most promising light sources for modern electronic devices and lighting systems. OLEDs are usually made of several layers of different organic materials, each layer having a specific function. Molecular complexes containing heavy metal atom, such as Pt or Ir, are regarded as one of the most promising materials for light-emitting layer of OLEDs because of their high efficiency and wavelength tunability. Theoretical and experimental research of such compounds is therefore crucial in development of OLED devices.

Here we present results based on quantum-chemical calculations of structural and electronic properties of bis(2-phenylbenzothiazole)-iridium-acetylacetonate ((pbt)<sub>2</sub>Ir(acac)) molecular complex and its derivatives. Molecular structure and excited-state properties of the compounds are determined using several computational models; the results are compared between the models and to the experimental data. The calculations were performed using *Gaussian03* and *GAMESS-US* programs.

The molecular structure of separate pbt ligand and the entire complex was optimized using density functional theory (DFT) with B3LYP functional and cc-pVDZ/lanl2DZ basis set, as well as model core potential approach with triple-zeta valence basis set (MCP-TZP, as implemented in *GAMESS-US*). The optimized geometries were in good correspondence to the results of similar theoretical studies, and moreover, the absorption spectra agreed fairly well with the experimental data. In addition to the ground-state structure (S<sub>0</sub>) geometry optimization of the lowest triplet state (T<sub>1</sub>), as well as calculations of the excited triplet states at both geometries were performed. Geometry optimization and excited states calculations of the extended ligand with additional carbazole groups and the resulting Ir complex were also carried out to assess the effect of carbazole groups to the wavefunction character of the lowest excited states of the complex.