**ΠΑΝΕΠΙΣΤΗΜΙΟ ΑΘΗΝΩΝ**
**ΤΟΜΕΑΣ ΦΥΣΙΚΗΣ ΣΤΕΡΕΑΣ ΚΑΤΑΣΤΑΣΗΣ**

**ΠΑΝΕΠΙΣΤΗΜΙΟΥΠΟΛΗ, 157 84 ΑΘΗΝΑ**

**ΕΘΝΙΚΟ ΜΕΤΣΟΒΙΟ ΠΟΛΥΤΕΧΝΕΙΟ**
**ΤΟΜΕΑΣ ΦΥΣΙΚΗΣ, ΣΧΟΛΗ ΕΦΑΡΜΟΣΜΕΝΩΝ ΜΑΘΗΜΑΤΙΚΩΝ ΚΑΙ ΦΥΣΙΚΩΝ ΕΠΙΣΤΗΜΩΝ**
**ΠΟΛΥΤΕΧΝΕΙΟΥΠΟΛΗ, 157 80 ΑΘΗΝΑ**

# ΣΕΜΙΝΑΡΙΟ
# ΦΥΣΙΚΗΣ ΣΥΜΠΥΚΝΩΜΕΝΗΣ ΥΛΗΣ

## Παρασκευή 24-11-2017 14:30 μ.μ.

Αίθουσα 027, Ισόγειο Κτηρίου Φυσικής, Πολυτεχνειούπολη Ζωγράφου

## "Modelling Nanomaterials Properties at the Atomic Level"

**Καθ. Παντελής Χ. Κελίρης**
*Τεχνολογικό Πανεπιστήμιο Κύπρου (ΤΕΠΑΚ)*

Agglomeration, crosslinking, buckling and other deformations of constituent units are processes that have a dramatic effect on the properties of nanomaterials, since they determine the nature of interfaces, junctions, edges and other discontinuities. Such processes are often ignored in theoretical descriptions and, instead, properties are inferred or projected by studying the ideal fundamental units and/or periodic arrangements of them. This is a severe limitation because deformations generate inhomogeneous fields, with certain areas/centers being more prominent and active than the rest of the nanostructure. Thus, for the elucidation of the macroscopic properties, the need for appropriate theoretical descriptors of local peculiarities arises. However, approaches able to describe nanomaterial properties at the local/atomic level are largely lacking from the state-of-the-art of the field. Here, we propose a general approach able to tackle this problem at various levels of sophistication. Its key element is the decomposition of macroscopic quantities into site contributions, which enables us to probe nanomaterial properties over a certain nanovolume. For the nano-optoelectronics, the crucial step is the decomposition of the frequency-dependent dielectric function. From this, the local absorption coefficient is obtained, as well as the conductivity and other relevant quantities. The method is demonstrated at the tight-binding (LCAO) level and in a first-principles DFT formalism. It is applied to two prototypical nanomaterials: Si nanocrystals/quantum dots embedded in a silica dielectric matrix and silver nanoparticles embedded in a diamond like carbon matrix.

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**Υπεύθυνοι Οργάνωσης Σεμιναρίου:**

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|---|---|---|---|
| Σ. Γλένης | Πανεπιστήμιο Αθηνών, | τηλ. 2107276811 | sglenis@phys.uoa.gr |
| Λ. Τσέτσερης | Ε. Μ. Π. | τηλ. 2107723046 | leont@mail.ntua.gr |