



The Department of Physics at the University of Cyprus
is organizing a seminar on

Thursday, 14 of September 2017, time 5:00 p.m.

Room B228, Building 13, New Campus

Speaker:

Professor Aristides D. Zdetsis

Molecular Engineering Laboratory, Department of Physics, University of Patras, Patras 26500 GR, Greece, & Institute of Electronic Structure and Laser, Foundation for Research & Technology Hellas, Vassilika Vouton, P.O. Box 1385, Heraklion, Crete GR-71110, Greece.

Present Address: Department of Physics University of Cyprus, Nicosia, CY

**“ Bridging the Physics and Chemistry of Graphene:
Electronic and Aromatic Properties of Graphene and
Graphene-Based Structures”**

Using a transparent methodology through a process of “spatial” evolution of properly constructed atomistic models with judiciously selected sizes and symmetries, we have obtained by real space ab initio Density Functional Theory (DFT) the “peculiar” aromatic and electronic properties of Graphene, as well as of various “nanographenes” (NGRs) and Polycyclic Aromatic Hydrocarbons (PAHs). This work leads naturally and almost effortlessly to a deep and fundamental Physical and Chemical understanding, not only of graphene itself, but also of graphene dots, anti-dots, PAHs, as well as atomically precise graphene nanoribbons (GNRs). For GNRs in particular, the present approach can bridge and rationalize the existing discrepancies in the literature for the size of the band gap, which could be as large as 300%.

For more information please contact:
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