MODELING OF 3D NANOGRAPHENE

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Recent efforts in graphene research include the realization of three-dimensional (3D) bulk materials with graphene nanoplatelets as their building blocks. These architectures are envisioned such as to retain the exceptional properties of 2D graphene in addition to providing mechanical robustness, high surface area and macroporosity; properties that are invaluable for a plethora of applications including catalysis, energy storage and conversion (carbon-based supercapacitors, electrodes in Li-ion batteries, active materials in solar cells), and as sensors, among others. In addition, the target to preserve high conductivity and electron mobility is essential for electronic applications.

In this talk, I present recent work in our group which is the first attempt to investigate the structural, mechanical and optoelectronic properties of realistic models of 3D nanographene (3D-NG). Our approach consists of Monte Carlo simulations for the generation of the 3D network, followed by tight-binding molecular dynamics simulations for full relaxation and calculation of the mechanical and optoelectronic properties. As starting constituents, we use graphene nanoplatelets of size 2-10 nm. The final 3D-NG structure is porous but rigid, with high surface area (~ 3000 m^2/g) and a density of about 0.5 gcm^{-3}. The nanoplatelets are curved, randomly oriented, interconnected and intertwined. About 90% of the atomic sites have sp^2 character. There are ~ 5% sp^3 sites, mainly at the junctions between the sheets, and ~ 5% sp^1 sites at the edges. There also are numerous small and large atomic rings. Despite this disorder, the electronic structure shows a large number of non-localized sp^2-like states at the Fermi level, giving rise to high conductivity of the order of 10^{-4} $\mu\Omega^{-1}cm^{-1}$, approaching that of single-layer graphene (within our methodology). Similarly, 3D-NG exhibits high absorption of the order of 10^5 cm^{-1} (in the visible). These properties make this 3D manifestation invaluable for applications in electronics and optics.

Short CV

Professor **P. C. Kelires** originates from the town of Akanthou, in Famagusta District. He is married and has three children. He got his B.Sc. degree (1981) in Physics from the University of Athens, Greece, and his Ph.D degree (1987) in theoretical Solid State Physics from the State University of New York, Albany (USA). He was IBM Research Division post-doctoral fellow at the world-renowned T. J. Watson Research Center, Yorktown Heights, New York (1987-89). He was elected as Assistant Professor in the Physics Department of the University of Crete (Greece) in 1989, and he got tenure as Associate Professor in 1994. He was promoted to full Professor in 2003. He was elected as Professor of Materials Science in the Cyprus University of Technology in 2006. He is internationally recognized as an expert in Computational Materials Science and Physics of Condensed Matter, especially in Monte Carlo simulations.

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