

A Molecular Description of Graphene: A Bridge from Benzene to Graphene Bridging its Chemistry and Physics

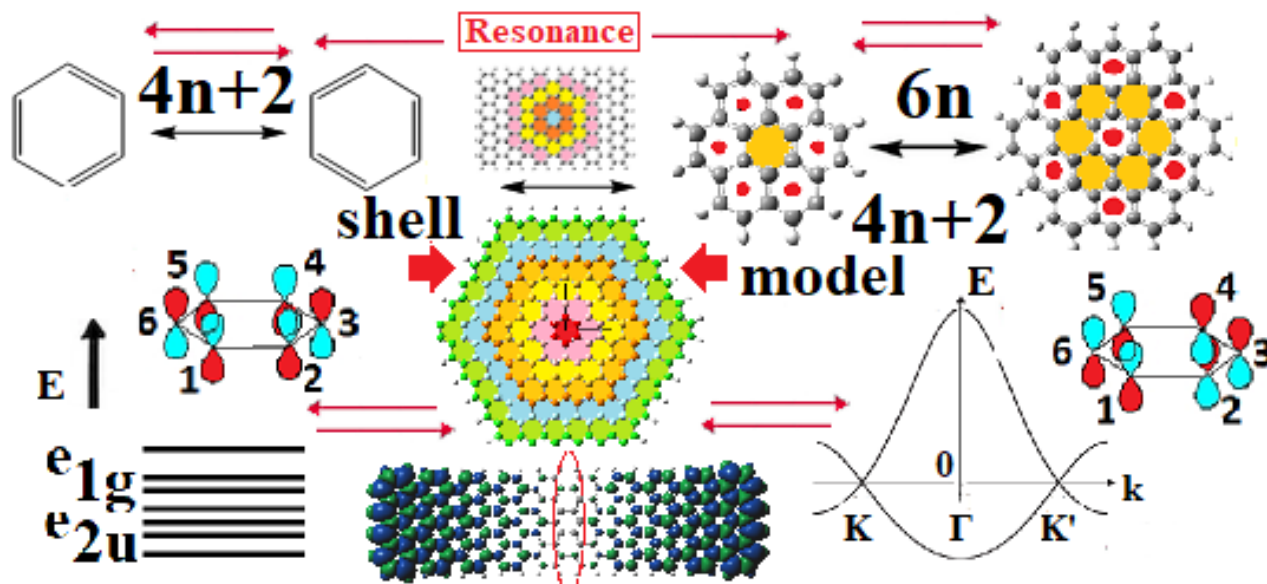
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Graphical Abstract



Abstract

The successful “molecular” description of graphene through a sequence of growing size polycyclic aromatic hydrocarbons (PAHs), not only serves as a bridge between the molecular and crystalline nature of graphene, but also at the same time links and interrelates in a transparent and comprehensive way the electronic and aromatic properties of benzene with those of graphene, revealing that graphene like benzene is a resonance structure, “resonating” between two complementary aromaticity patterns [1-2]. Thus, graphene is the prototypical aromatic “crystal” in full analogy to benzene which is the prototypical aromatic molecule. The two are connected through aromaticity, which is proven a very useful, simple, and transparent “everyday” tool, rather than a

remote and “suspicious” concept [3]. The underlying fundamental linking property is the shell model (or shell structure), which can be visualized as a babushka-like Russian doll in which the PAHs of the main sequence [1] comprising the benzene-to-graphene bridge are stuck one inside the other. Through the shell model we can rationalize the two fundamental (but empirical) rules of aromaticity, Hückel’s and Clar’s, and establish their (topological) interconnection through the “shell model”. The shell structure, initially generated by hexagonal PAHs is fully operative in rectangular (D_{2h} , and other symmetries) offering novel and vital understanding of the electronic properties of graphene nanoribbons (GNRs). Such understanding includes, among others, the $3n/3n\pm 1$ width rule for GNRs, as well as edge magnetism, which, if any, should not originate from real spin, but rather from pseudospin represented by the orientation of the atomic p_z orbitals in the particular lattice site, which is fully determined by symmetry, and in particular by inversion symmetry. It is shown that inversion symmetry conflict in armchair GNRs (AGNRs) is responsible for the generation of zigzag edge states in AGNRs, which appear to be a subtle point in the experimental determination of the band gap in atomically precise AGNRs, in particular of the very narrow ones, together with other uncertainties [5]. On the other hand, we find that inversion symmetry conflict, which in the many-body theory of graphene leads to inversion (and parity) symmetry breaking, is responsible for the Dirac points of graphene, at the K points in the standard band structure which represents an “average picture” in relation to the “dynamical” picture of the present work, created by the spatial evolution of the hexagonal PAHs of the “main sequence” underlying the shell model [1]. Finally, in this work, through the shell model and simple symmetry arguments, a new simple, transparent and powerful geometrical notion of aromaticity is revealed, which can be used as a “casual” modern tool, despite its past history and “suspicious behavior” [3], which coupled with simple symmetry arguments can lead to very rich, transparent, and insightful results, many of which could be obtained only by advanced techniques such as many-body and/or Chemical graph theory. The present approach should be also useful for other “honeycomb”-based structures, sharing the common feature of “alternant” or “bipartite” topology.

Keywords: Graphene; polycyclic aromatic hydrocarbons; aromaticity; nano graphene; graphene nanoribbons.

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Biography of Presenting Author



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Research Activities

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There are more than 60 presentations in Greek and international conferences (many of which are invited).

Books

1. "Quantum Physics I" I» (pages 550) in Greek, Hellenic Open University (2004). ISBN: 960-538-626-7
2. "Vibrations and Waves" (pages 377 Volume I) in Greek, Hellenic Open University (2004). ISBN: 960-538-629-1
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5. "From Benzene to Graphene: Bridging The Physics and Chemistry of Graphene" 2020 (pending Publishing Agreement)

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