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Understanding and optimizing alternant and non-alternant nanographenes for spintronic and optoelectronic applications

Abstract: Motivated by the recent synthesis of non-alternant isomers of small peri acenes (seen as short armchair nanoribbons, AGNRs, with Z=3, 4 zigzag rings, and A=2 armchair rings) through the introduction of Stone-Wales (SW) and "SW-like" (azulene) moieties, on their alternant isomers (AGNRs), we set here to examine the roots, and profound characteristics of such nanographenes (NGRs or SW-AGNRs) to systematically optimize and functionalize their spintronic and optoelectronic properties. Although decreasing antiaromaticity determines the spin state for a given geometry, increasing aromaticity is the decisive factor for selecting the ground state geometry. Yet, it is not necessarily associated with larger negative values or negligible positive numbers of nucleus-independent chemical shifts (NICS). Actually, "higher aromaticity" may be accompanied by highly antiaromatic rings with positive NICS numbers. It is demonstrated that "increasing aromaticity" in fact describes the topological capability of the non-alternant system to accommodate the full (or the largest part of the) aromaticity pattern of the corresponding alternant NGR, meaning that "defects" should be concentrated as much as possible around the empty rings. The aromaticity pattern is fully determined by the number Z of zigzag rings at the two ends. We suggest that the optimum NGRs are the SW3x4 which is optimum for spintronic applications (but not for optoelectronic applications) and the SW4x4 which is suitable for both. These results and conclusions are in accord with earlier predictions of the present author about the "topological/aromatic" role of "empty" rings. Furthermore, they are also validated by the already synthesized non-alternant NGRs

Keywords: Carbon Nanostructures, Graphene, Magnetic Materials, Materials-Chemistry, Non-alternant nanographenes.

Biography: Aristides D. Zdetsis, Professor Emeritus department of Physics University of Patras, director Molecular engineering Laboratory. The focus of my work for the last ten years is on graphene, graphene-like graphene structures, 2D-materials and non-benzenoid materials with applications in spintronics (molecular magnetism), and optoelectronics. I am an IAAM and a VEBLEO fellow. I have written more than 150 research papers, and I have made more than 300 verified reviews (web of science) in major scientific journals, funding agencies and faculty promotions. I am listed in the top 2% of scientists worldwide in Stanford List, or 0.5% in Scholar GPS, with h=31.

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