NanoLab Talk

Politecnico di Milano, Department of Energy, Cesnef (Building 19), via Ponzio 34/3, Milan

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# Recent advances on sp-carbon nanostructures: modeling of structural, electronic and vibrational properties


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Carbon-atom wires (CAWs) are linear, finite-length molecules, whose ideal limit is the so-called "carbyne [1]. Similar to other polyconjugated systems, CAWs display structural, electronic and optical properties which can be tuned by their length and by the nature of the end-groups, offering an appealing opportunity for developing novel functional nanostructures. In addition, 2D hybrid sp-$sp^2$ carbon nanostructures, such as graphdiynes (GDY), shows structure-dependent properties which can be properly designed to tune the semiconductor to metal transition. Focusing on CAWs terminated by different end-groups, Density Functional Theory is here employed to predict the molecular structure, the electronic gap, and the Raman response as a function of the chain structure and/or the occurrence of charge transfer, also comparing calculations with experimental data. CAWs terminated by different $sp^2$ moieties are discussed to highlight the role of end-groups on π-electron delocalization; then, the occurrence of charge transfer with metal nanoparticles is taken into account to analyze SERS spectra of selected systems [2]. Donor/acceptor CAWs are then investigated to reveal how charge transfer is modulated by both the sp-carbon chain length, and peculiar functional groups [3]. Finally, confinement in 2D γ-GDY and related nanoribbons is computationally investigated to reveal the effect of topology and edge-type on the band gap and on the vibrational response [4]. These results provide guidelines for the design of novel nanostructures based on CAWs, including also sp-$sp^2$ hybrid systems where graphene-like and polyyne-like domains are closely interconnected

**References**


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[2] A. Milani et al., J. Phys. Chem. C 2017, 121, 10562

[3] A. Milani et al. Scientific Reports 2019, 9, 1648

[4] P. Serafini et al. Phys. Rev. Mater. 2020, 4, 014001


**About the speaker:**

Alberto Milani graduated in Materials Engineering in 2005 at Polytechnic of Milan, where, in 2009, he got also a PhD in Materials Engineering. His research activity focuses on the quantum chemical computational investigation of molecular interactions in polyconjugated materials, polymers and hydrogen-bonded complexes. In particular, his main research focus is the interpretation of vibrational (IR/Raman) spectra and the understanding of structure/properties. He published more than 75 papers or reviews on international peer-reviewed journals.


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