Electronic transport in 1D atomic carbon chains and in 2D conjugated polymer networks

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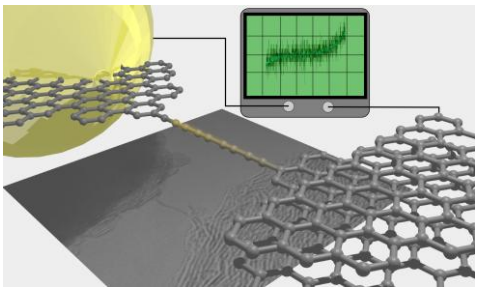

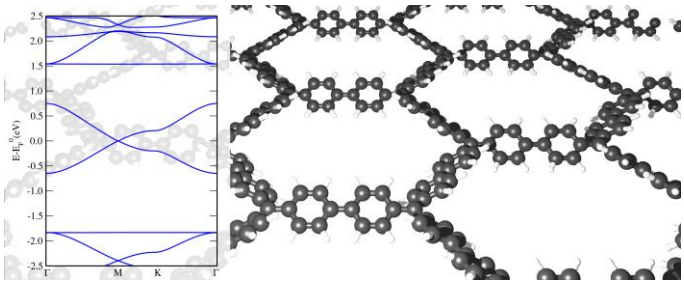

Carbyne, the sp^1-hybridized phase of carbon, is still a missing link in the family of carbon allotropes. Recently, detailed electrical measurements and first-principles electronic transport calculations have been performed on monoatomic carbon chains [1]. When the 1D system is under strain, the current-voltage curves exhibit a semiconducting behavior, which corresponds to the polyyne structure of the atomic chain with alternating single and triple bonds. Conversely, when the chain is unstrained, the ohmic behavior is observed in agreement with the metallic cumulene structure with double bonds. These measurements confirm recent theoretical predictions, namely that a metal-insulator transition can be induced by adjusting the strain in carbyne [2]. The key role of the contacting leads is also scrutinized by *ab initio* quantum conductance calculations, explaining the rectifying behavior measured in monoatomic carbon chains in a non-symmetric contact configuration.

Two-dimensional conjugated polymers exhibit electronic structures analogous to that of graphene with the peculiarity of π–π^* bands which are fully symmetric and isolated. Realistic 2D conjugated polymer networks with a structural disorder such as monomer vacancies (unavoidable during bottom-up synthesis) are investigated using both *ab initio* and *tight-binding* techniques in order to check their suitability for electronic applications. As expected, long mean free paths and high mobilities are predicted for low defect densities. At low temperatures and for high defect densities, strong localization phenomena originating from quantum interferences of multiple scattering paths are observed in the close vicinity of the Dirac energy region while the absence of localization effects is predicted away from this region suggesting a sharp mobility transition [3].

[1] ***Electrical transport measured in atomic carbon chains***
O. Cretu, A. R. Botello-Méndez, I. Janowska, C. Pham-Huu, J.-C. Charlier, and F. Banhart
Nano Letters **13**, 3487-3493 (2013).

[2] ***Strain-induced metal-semiconductor transition observed in atomic carbon chains***
A. La Torre, A. R. Botello-Méndez, W. Baaziz, J.-C. Charlier, and F. Banhart
Nature Communications **6**, 6636 (2015).

[3] ***The electronic and transport properties of 2D conjugated polymer networks including disorder***
J.-J. Adjizian, A. Lherbier, S.M.-M. Dubois, A.R. Botello-Méndez, and J.-C. Charlier
Nanoscale **8**, 1642 (2016).