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Ab initio quantum transport in atomic carbon chains ANDRÉS R. BOTELLO-MÉNDEZ, JEAN-CHRISTOPHE CHARLIER, University of Louvain, Institute of Condensed Matter and Nanosciences (Belgium), FLORIAN BANHART, Université de Strasbourg, Institut de Physique et Chimie des Matériaux (France), NAPS TEAM, CARBYNE COLLABORATION — Carbyne, the *sp*-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, confirming recent theoretical predictions, namely that a metal-insulator transition can be induced by adjusting the strain. The key role of the contacting leads is also scrutinized by *ab initio* quantum conductance calculations [2], explaining the rectifying behavior measured in monoatomic carbon chains in a non-symmetric contact configuration.

[1] O. Cretu, A. R. Botello-Mendez, I. Janowska, C. Pham-Huu, J.-C. Charlier, and F. Banhart, Nano Lett. 13, 3487-3493 (2013).
[2] A. La Torre, A. R. Botello-Mendez, W. Baaziz, J.-C. Charlier, and F. Banhart, submitted for publication (2014).

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