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NanoLab

NanoLab Talk

Tuesday, 13th october, 2018 – 11.30

Seminar Room 1° floor

Department of Energy – Cesnef (Building 19) via Ponzio 34/3 Milan

Politecnico di Milano

"Cumulenes and polyynes as carbon atomic wires"

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Abstract:

Oligoynes, polyynes, and cumulenes (constructed of sp-hybridized carbon, known as carbon atomic wires – CAWs) are arguably the simplest molecular wires. In addition to their and semi-rigid structure, electronic delocalization through the conjugated framework is essentially unaffected by bond rotation, which separates CAWs from nearly all other wire motifs. While shorter CAWs are reasonable stable and easy to study, longer CAWs are often chemically unstable, which renders them inefficient for device formation. Thus, the development of synthetic routes that provide stable molecules for incorporation into devices is necessary in order to answer questions related to the performance of CAWs.

Our recent work has targeted three major challenges regarding CAWs, including 1) The synthesis of polyyne[1] and cumulene[2] CAWs to model carbyne (the sp-hybridized carbon allotrope), 2) The study of structural aspects of CAWs, and 3) Synthetic approaches to stabilize CAWs for devices.[3] For example, pyridyl endgroups have been designed with sterically demanding substituents that protect the CAWs, while maintaining access of the pyridyl nitrogen to the electrodes. Alternative, we use supramolecular chemistry to form rotaxanes in which the linear polyyne is threaded through a macrocycle, forming the equivalent of an insulated molecular wire. Third, we use the pyridyl nitrogen to coordinate to transition metals, which provides alternative structures for molecular wires. The use of CAWs in single molecule devices ultimately helps to provide an answer to the question of performance based on structure and length.

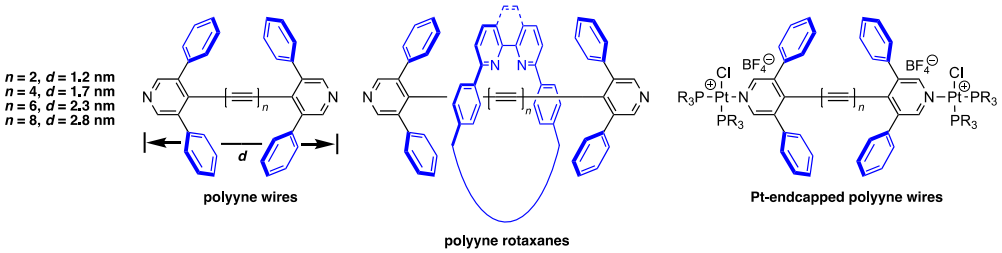

Figure 1. Examples of pyridyl endcapped CAWs for devices.

References

[1] W.A. Chalifoux, R.R. Tykwinski, *Nat. Chem*. **2010**, *2*, 967–971.

[2] J.A. Januszewski, R.R. Tykwinski, *Chem. Soc. Rev*. **2014**, *43*, 3184–3203.

[3] D.C. Milan, M. Krempe, A.K. Ismael, L.D. Movsisyan, M. Franz, I. Grace, R.J. Brooke, W. Schwarzacher, S.J. Higgins, H.L. Anderson, C.J. Lambert, R.R. Tykwinski, R.J. Nichols, *Nanoscale* **2017**, *9*, 355–361.

About the speaker:

Rik R. Tykwinski earned his BS at the University of Minnesota – Duluth (1987) and his PhD the University of Utah with Professor Peter Stang (1994). As a PDF at ETH-Zürich, he worked with Professor François Diederich, and in 1997 he joined the faculty at the University of Alberta. In 2009, he moved to Germany to accept the position of Chair of Organic Chemistry at the University of Erlangen-Nürnberg, and in 2016 he moved back to Alberta as Chair of the Department of Chemistry. He is a physical organic chemist, with a focus on structure-property relationships in conjugated molecules, especially polyynes and cumulenes. In his free time, he enjoys mountain biking and entertaining his sons.

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