

1D and 2D networks of cyclo-paraphenylenes (CPPs) using covalent and self-assembly process by DFT

J. Rio¹ D. Erbahar² P. Briddon³ N. Tagmatarchis⁴ H. A. Wegner⁵ C. Ewels¹

¹Institut des Matériaux Jean Rouxel (IMN), Université de Nantes, CNRS UMR 6502, F-44322 Nantes, France

²Physics Department, Gebze Technical University, Gebze, Turkey

³School of Electrical and Electronic Engineering, University of Newcastle, Newcastle upon Tyne, NE 1 7RU, UK

⁴Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, Athens, Greece

⁵Institute of Organic Chemistry, Justus Liebig University, Heinrich-Buff-Ring 17, 35392 Giessen, Germany

Cycloparaphenylenes (CPPs) represent the shortest possible segment of (n,n) armchair carbon nanotubes (CNTs), and as such may represent a new route to producing chirally selected carbon nanotubes [1] [2]. Current approaches for this envisage controlling synthesis of uniform-diameter single chirality CNTs using CPPs as templates, which has met with limited success [3]. At the same time complexes of fullerenes with CPPs have been reported, highlighting a high size selectivity of the CPPs to the specific fullerene.

In the current study we explore a new approach, namely using covalent- and non-covalent self-assembly of either functionalized CPPs, or CPP-C₆₀ hybrid systems, to create new types of poly-CPP-nanotubes. These new materials, while also adopting a controlled chirality tubular morphology, show distinctly different chemical, mechanical, electronic and optical behavior to conventional carbon nanotubes.

The first of these families involves chemical cross-linking between neighbouring CPPs using fullerenes as alignment templates. The resultant poly-CPP-nanotubes share some properties with conjugated polymers, notably the ability to add functionality and control electronic properties through functionalisation control. The second family using self-assembly stacking between C₆₀ and different sizes of [6]-, [8]-, [10]-CPPs to form 1D and 2D networks. While the study is driven by our theoretical modelling, we successfully demonstrate via a joint experimental-theoretical study the first steps towards their production, namely trapping of 2CPP rings around a fullerene dimer (C₅₉N)₂ [4].

[1] A.-F. Tran-Van, E. Huxol, J. M. Basler, M. Neuberger, J.-J. Adjizian, C. P. Ewels and H. A. Wegner, *Org. Lett.* **16**, 1594-1597 (2014).

[2] J. Rio, D. Erbahar, M. Rayson, P. Briddon and C. P. Ewels, *Phys. Chem. Chem. Phys.* **18**, 23257-23263 (2016).

[3] H. Omachi, T. Nakayama, E. Takahashi, Y. Segawa and K. Itami, *Nat. Chem.* **5**, 572-576 (2013).

[4] J. Rio, S. Ahles, C. Ewels, D. Jacquemin, N. Tagmatarchis, H. A. Wegner, *in preparation* . (2017).