Impact of side group functionalisation in the charge transport properties of graphene-curcuminoids single-molecule devices

Rossella Zaffino

Thomas Y. Baum,[b] Teresa Cardona-Lamarca,[a] Daniel Herrera,[a] Raphael Pfattner,[a] Silvia Gómez-Coca,[c,d] Eliseo Ruiz,[c,d] Arántzazu González-Campo,[a] Herre S. J. van der Zant [b] and Núria Aliaga-Alcalde[a,e]

[a] *ICMAB-CSIC (Institut de Ciència dels Materials de Barcelona), Campus de la Universitat Autònoma de Barcelona, 08193 Bellaterra, Spain*
[b] *Kavli Institute of Nanoscience, Delft University of Technology, Lorentzweg 1, 2628 CJ Delft, The Netherlands*
[c] *Departament de Química Inorgànica i Orgànica, Universitat de Barcelona, C/Martí i Franqués 1-11, 08028 Barcelona, Spain*
[d] *Institut de recerca de Química Teòrica i computacional, Universitat de Barcelona, Diagonal 645, 08028 Barcelona, Spain*
[e] *ICREA (Institució catalana de Recerca i Estudis Avançats), Passeig Lluís Companys 23, 08018 Barcelona, Spain*

rzaffino@icmab.es

The ability to control charge transport in a single-molecule junction is relevant for the analysis of fundamental aspects of quantum transport through a molecule, as well as for the design of advanced functional molecular electronic devices. In this regard, the role of interface engineering proves to be fundamental in controlling the transport mechanism in single-molecule transistors[1]. Carbon-based electrodes, unlike standard metals, offer the possibility of exploiting both covalent bonding and π-π stacking to the electrodes. However, covalent bonding could negatively interfere by breaking the extended π conjugation intrinsic to both systems. For this reason, supramolecular functionalisation via π-π stacking is usually explored in experimental studies and, so far, mainly families of small polycyclic aromatics have been used. In this work, we analyse the transport properties of single-molecule junctions using linear diarylheptanoid (CCMoids) embedded between graphene nano-gap electrodes fabricated by feed-back controlled electro-burning. We explored two different backbone functionalisation strategies: adding anthracene anchoring groups[2] and introducing a spacer amide bond between the conjugate chain and the considered anchoring group (pyrene). The results obtained are compared with those observed in the past with related CCMoids.[3] In all the cases, we were able to demonstrate gate-dependent transport, at room and low temperatures. We found higher conductance values for the longest system studied which we attributed, according to the DFT calculation, to the fully planar configuration of the molecule within the junctions favoured by the presence of the amide bond.

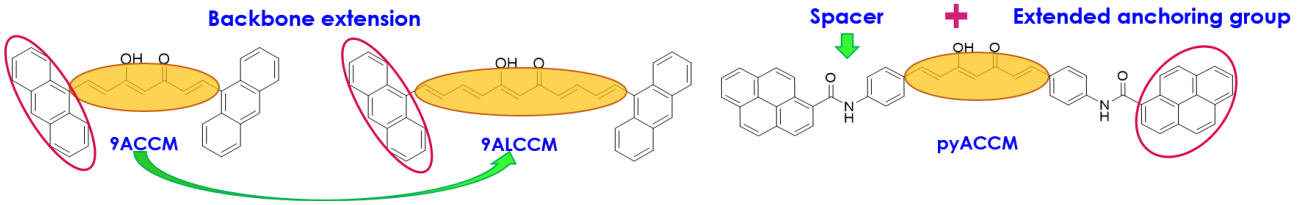

Figure1. From left to right: Chemical structures of 9ACCM, 9ALCCMoid and pyACCM.

References

[1] Chen *et al.* **2024**. https://doi.org/10.1002/anie.202401323.
(2) Prins *et al.* Room-Temperature Gating of Molecular Junctions Using Few-Layer Graphene Nanogap Electrodes. *Nano Lett.* **2011**, *11* (11), 4607–4611. https://doi.org/10.1021/nl202065x.
[3] Burzurí *et al.* Sequential Electron Transport and Vibrational Excitations in an Organic Molecule Coupled to Few-Layer Graphene Electrodes. *ACS Nano* **2016**, *10* (2), 2521–2527. https://doi.org/10.1021/acsnano.5b07382.