Engineering of Charge Current Flow in Nanoporous Graphenes

Isaac Alcón, Gaetano Calogero, Nick Papior, Aleandro Antidormi, Aron Cummings, Mads Brandbyge and Stephan Roche

Catalan Institute of Nanoscience and Nanotechnology (ICN2), Campus UAB, Bellaterra, 08193 Barcelona, Spain
isaac.alcon@icn2.cat

During the last decade, on-surface fabricated graphene nanoribbons (GNRs) have gathered enormous attention due to their semiconducting π-conjugated nature and atomically precise structure.[1] GNRs are regularly characterized by means of scanning probe microscopy (SPM), which has also allowed to study exotic electronic quantum phases realized in these nanostructured materials.[2] A significant breakthrough in the same field was the recent fabrication at ICN2 of nanoporous graphene (NPG) as a 2D array of laterally bonded GNRs.[3] This covalent integration of GNRs could enable complex electronic functionality at the nanoscale, with the ability to tune the electronic coupling between GNRs within NPGs. In this talk, I will present our recent works, based on quantum chemical calculations and large-scale transport simulations, and in which we demonstrate unprecedented electronic control of NPG either through a rational chemical design[4] or by external means such as electrostatic gates (**Fig. 1a**).[5] Our simulations of local injection of currents in NPGs evidence the control capability of spatial current distribution with sub-nanometer precision (**Fig. 1b-c**), results which could be experimentally probed using SPM. Our most recent studies also generalize these ideas to other types of carbon nanostructures[6] and, importantly, their applicability at finite temperature. A fundamental strategy to design carbon nanodevices with built-in externally tunable electronics and spintronics is thus proposed, and should be key for future applications such as bio-chemical nanosensing and carbon nanoelectronics.

References

[1] J. Cai, P. Ruffieux, R. Jaafar, M. Bieri, T. Braun, S. Blankenburg, M. Muoth, A. P. Seitsonen, M. Saleh, X. Feng, K. Müllen, R. Fasel, *Nature* 466 (2010) 470
[2] D. J. Rizzo, G. Veber, T. Cao, C. Bronner, T. Chen, F. Zhao, H. Rodriguez, S. G. Louie, M. F. Crommie and F. R. Fischer, *Nature*, 2018, 560, 204–208
[3] C. Moreno, M. Vilas-Varela, B. Kretz, A. Garcia-Lekue, M. V. Costache, M. Paradinas, M. Panighel, G. Ceballos, S. O. Valenzuela, D. Peña, A. Mugarza, *Science* 360 (2018) 199
[4] G. Calogero, I. Alcón, N. Papior, A.P. Jauho and M. Brandbyge, *JACS*, 2019, 141, 13081–13088
[5] I. Alcón, G. Calogero, N. Papior and M. Brandbyge, *Adv. Funct. Mater.*, 2021, 31, 2104031
[6] I. Alcón, G. Calogero, N. Papior, A. Antidormi, K. Song, A. Cummings, M. Brandbyge and S. Roche "Multiradical character of biphenylene and its anisotropic charge transport". Submitted to *JACS*

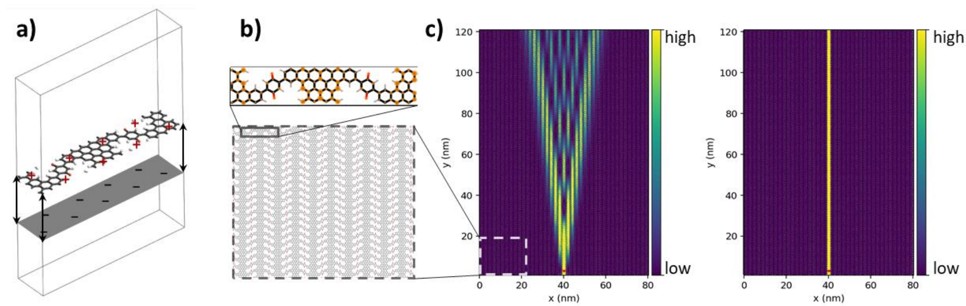

Figure 1: (**a**) Periodic unit cell of an electrostatically gated (gray plane) newly designed NPG, where GNRs are connected via aryl-quinone units. (**b**) Construction of large-scale NPG devices. (**c**) Spreading of currents (maximum magnitude in yellow) locally injected at the bottom of large-scale NPG devices (see red dot) at different applied gates (as outlined in **a**).