

Graphene-PVC composites through exfoliation in low boiling point solvents with Perylenediimides

Konstantinos Kouroupis-Agalou^{1,2}, Elias Gebremedhn³, Andrea Liscio¹, Mohamed El Garah⁴, Wassima Rekab⁴, Artur Ciesielski⁴, Massimo Gazzano², Vittorio Morandi⁵, Paolo Samori⁴, David Beljonne³, Vincenzo Palermo¹

¹ *Istituto per la Sintesi Organica e la Fotoreattività-Consiglio Nazionale delle Ricerche (ISOF-CNR), Bologna, Italy.*

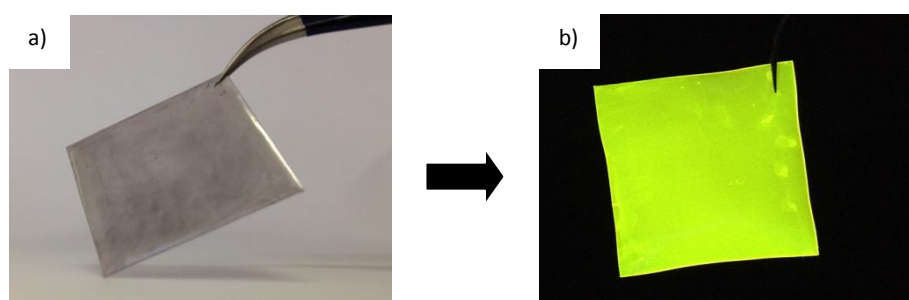
² *Department of Chemistry "Giacomo Ciamician", University of Bologna, Bologna, Italy.*

³ *Laboratory for Chemistry of Novel Materials, University of Mons, Mons, Belgium.*

⁴ *ISIS & icFRC, Université de Strasbourg & CNRS, Strasbourg, France.*

⁵ *Istituto per la Microelettronica e Microsistemi-Consiglio Nazionale delle Ricerche (IMM-CNR), Bologna, Italy.*

Perylenediimides (PDIs) are key building blocks in modern organic (opto)electronics due to their excellent photophysical and electrical properties¹. We demonstrate that these dyes can be used to successfully exfoliate graphite to produce graphene sheets, not only in the typical high-boiling point solvents like DMF (dimethylformamide) or NMP (N-methyl-2-pyrrolidone), but also in low-boiling point ones such as THF (tetrahydrofuran) and CHCl₃ (chloroform). The functionalization of PDI molecules with phenylethyl side groups exposing -H, -F, -Cl was also explored. A combination of microscopic, spectroscopic and modeling techniques are employed in order to gain a multiscale understanding on the physical and chemical properties of the bi-component material. The physisorption of the different PDIs on graphite, forming highly ordered 2D supramolecular architectures, is explored at the molecular scale by scanning tunneling microscopy (STM) and molecular dynamics (MD) simulations. Such densely packed adlayer plays an important role in boosting the graphene exfoliation efficiency. PDI/liquid-phase exfoliated graphene blends revealed a variation in the electrical performances of 2- and 3- terminal devices depending on the molecular functionalization (-H, -F, -Cl). Finally, we demonstrate an original approach to include the exfoliated material onto a polyvinylchloride (PVC) film surface to create a conductive graphene-based hybrid nanocomposite.



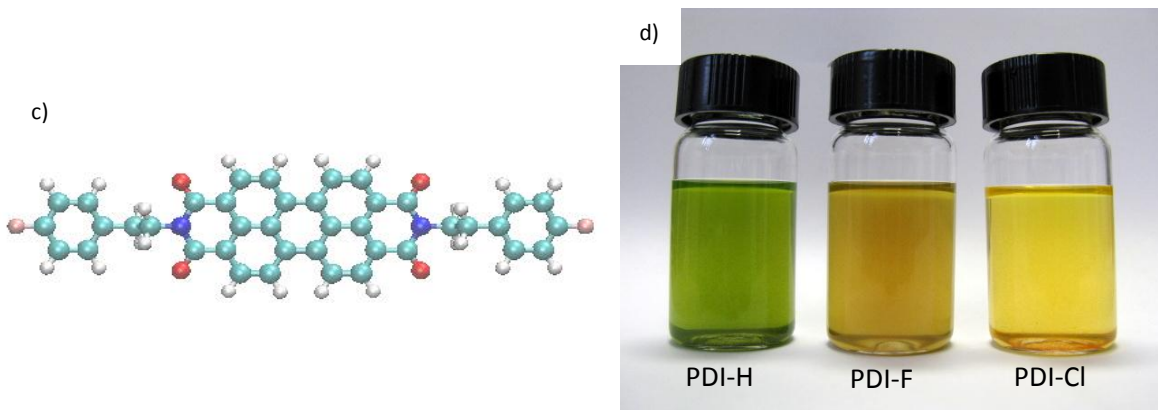


Fig: a) PVC membrane treated in graphene-PDI suspension, b) the same membrane under UV lamp, revealing the presence of uniformly dispersed molecules, c) molecular structure of PDI, d) PDI-derivatives with different side groups functionalization (-H, -F, -Cl) dispersed in THF solvent.

References:

- [1] A. Schlierf, k. Cha, M. G. Schwab, P. Samori, V. Palermo, 2D Materials, 1, (2014).