Polyaromatic cores for the exfoliation of popular 2D materials

Electronic Supplementary Information

Marina Garrido^{a,*}, Myriam Barrejón^{a,b}, José Augusto Berrocal^c, Zois Syrgiannis^{a,d}, Maurizio Prato^{a, e, f}

^a Department of Chemical and Pharmaceutical Sciences, INSTM UdR Trieste, Università degli Studi di Trieste, Via Licio Giorgieri 1, Trieste 34127, Italy

^b Neural Repair and Biomaterials Laboratory, Hospital Nacional de Parapléjicos (SESCAM), Finca la Peraleda s/n, 45071 Toledo, Spain.

^c Adolphe Merkle Institute, University of Fribourg, Chemin des Verdiers 4, 1700 Fribourg, Switzerland

^d Simpson Querrey Institute for BioNanotechnology, Northwestern University, Chicago, IL 60611, USA; Departement of Chemistry, Northwestern University, Evanston, IL 60208, USA.

 ^e Center for Cooperative Research in Biomaterials (CIC biomaGUNE), Basque Research and Technology Alliance (BRTA), Paseo de Miramón 194, Donostia-San Sebastián 20014, Spain
^f Ikerbasque, Basque Foundation for Science, Bilbao 48013, Spain

*Corresponding author: mgarrido@units.it

Supplementary figures



Figure S1. Schematic representation of the exfoliation method.



Figure S2. Image of the biphasic systems after the exfoliation process. In the upper part are shown graphite, $g-C_3N_4$, BN and MoS_2 in the presence of C_{10} -NDI- C_{10} . In the bottom part are shown graphite, $g-C_3N_4$, BN and MoS_2 in the presence of C_{10} -PDI- C_{10} . In blue is marked the level of the organic phase (DCM) and in red the level of the aqueous phase.



Figure S3. TEM images of a) graphene and d) MoS_2 exfoliated in the presence of C_{10} -NDI- C_{10} , b) g- C_3N_4 and c) BN exfoliated in the presence of C_{10} -PDI- C_{10} . The scale bares are 500 nm for graphene, 200 nm for g- C_3N_4 , 100 for BN and 20 nm for MoS_2 .



Figure S4. TEM images of a) graphene, b) g-C₃N₄, c) BN and d) MoS₂ exfoliated in the absence of the aromatic molecules C_{10} -NDI- C_{10} or C_{10} -PDI- C_{10} . The scale bares are 200 nm for graphene, g-C₃N₄, BN and 100 nm for MoS₂.



Figure S5. Exfoliation of graphene. Upper part) Representative AFM image, corresponding height profile and statistical analysis showing the thickness of graphene exfoliated in the presence of C_{10} -NDI- C_{10} . Lower part) Representative AFM image, corresponding height profile and statistical analysis showing the thickness of graphene exfoliated in the presence of C_{10} -PDI- C_{10} .



Figure S6. Exfoliation of $g-C_3N_4$. Upper part) Representative AFM image, corresponding height profile and statistical analysis showing the thickness of $g-C_3N_4$ exfoliated in the presence of C_{10} -NDI- C_{10} . Middle part) Representative AFM image, corresponding height profile and statistical analysis showing the thickness of $g-C_3N_4$ exfoliated in the presence of C_{10} -PDI- C_{10} . Lower part) Representative AFM image, corresponding height profile and statistical analysis showing the thickness of $g-C_3N_4$ exfoliated in the absence of the aromatic cores.



Figure S7. Exfoliation of BN. Upper part) Representative AFM image, corresponding height profile and statistical analysis showing the thickness of BN exfoliated in the presence of C_{10} -NDI- C_{10} . Middle part) Representative AFM image, corresponding height profile and statistical analysis showing the thickness of BN exfoliated in the presence of C_{10} -PDI- C_{10} . Lower part) Representative AFM image, corresponding height profile and statistical analysis showing the thickness of BN exfoliated in the presence of C_{10} -PDI- C_{10} . Lower part) Representative AFM image, corresponding height profile and statistical analysis showing the thickness of BN exfoliated in the absence of the aromatic cores.



Figure S8. Exfoliation of MoS₂. Upper part) Representative AFM image, corresponding height profile and statistical analysis showing the thickness of MoS₂ exfoliated in the presence of C_{10} -NDI- C_{10} . Middle part) Representative AFM image, corresponding height profile and statistical analysis showing the thickness of MoS₂ exfoliated in the presence of C_{10} -PDI- C_{10} . Lower part) Representative AFM image, corresponding height profile and statistical analysis showing the thickness of MoS₂ exfoliated in the presence of C_{10} -PDI- C_{10} . Lower part) Representative AFM image, corresponding height profile and statistical analysis showing the thickness of MoS₂ exfoliated in the presence of C_{10} -PDI- C_{10} . Lower part) Representative AFM image, corresponding height profile and statistical analysis showing the thickness of MoS₂ exfoliated in the absence of the aromatic cores.

The statistical analyses were performed on at least 70 sheets for each exfoliated material in the presence of the aromatic molecules. In the case of the exfoliation in the absence of the aromatic cores, the statistical analyses were performed on at least 20 sheets for each material.



Figure S9. Average Raman spectra ($\lambda_{exc} = 532$ nm) of commercial graphite (black) and expanded graphite (red).



Figure S10. Average Raman spectrum ($\lambda_{exc} = 633$ nm.) of expanded graphite.



Figure S11. Average Raman spectra ($\lambda_{exc} = 633 \text{ nm}$) of graphene exfoliated in the presence of C₁₀-PDI-C₁₀ (red) and in its absence (black). Detailed inset of the 2D band and its deconvolution.



Figure S12. Average Raman spectrum ($\lambda_{exc} = 633 \text{ nm}$) of bulk g-C₃N₄. Enlarged Raman spectrum of the region located between 670 and 740 cm⁻¹.



Figure S13. Average Raman spectra ($\lambda_{exc} = 633$ nm) of g-C₃N₄ exfoliated in the presence of C₁₀-PDI-C₁₀ (red) and in its absence (black). Enlarged Raman spectra of the region located between 670 and 740 cm⁻¹.



Figure S14. A) Average Raman spectrum of bulk BN ($\lambda_{exc} = 633$ nm). B) Average Raman spectrum of bulk BN ($\lambda_{exc} = 532$ nm).



Figure S15. Average Raman spectra ($\lambda_{exc} = 532 \text{ nm}$) of BN exfoliated in the presence of C₁₀-PDI-C₁₀ (red) and in its absence (black). In purple is marked the FWHM.



Figure S16. Average Raman spectrum of bulk MoS_2 ($\lambda_{exc} = 785$ nm).



Figure S17. Average Raman spectra ($\lambda_{exc} = 785 \text{ nm}$) of MoS₂ exfoliated in the presence of C₁₀-PDI-C₁₀ (red) and in its absence (black).



Figure S18. UV-Vis spectra in DCM of C_{10} -PDI- C_{10} (black), graphene PDI (red), g- C_3N_4 PDI (blue), BN PDI (green) and MoS₂ PDI (purple).



Figure S19. ¹H-NMR of **C**₁₀-**NDI-C**₁₀ (400 MHz, CDCl₃).



Figure S20. ¹H-NMR of C_{10} -PDI- C_{10} (400 MHz, CDCl₃).