Supplementary information file

Electronic interaction and work function tuning investigation of phthalocyanines molecules and graphene interfaces.

Yunier Garcia-Basabe,[a,] Matheus Suenson Cardoso,[b,d] Bruno da Silva Lima,[b] Cesar D. Mendoza,[c,e] Fernando Lázaro Freire Junior,[c] and Dunieskys G. Larrude,[b,*].*

[a.] *Universidade Federal da Integração Latino-Americana, UNILA, 85867-970, Foz do Iguaçu, Brazil.*
[b.] *School of Engineering, Mackenzie Presbyterian University, São Paulo 01302-907, Brazil.*
[c.] *Department of Physics, Pontifícia Universidade Católica do Rio de Janeiro, 22451-900, Rio de Janeiro, Brazil.*
[e.] *Present address: Department of Electrical Engineering, Universidade do Estado do Rio de Janeiro, 20550-900, Rio de Janeiro, Brazil.*
[d.] *School of Physics and Astronomy, University of Manchester, Manchester M13 9PL, U.K.*

** Corresponding author:*
Email: yunier.basabe@unila.edu.br
yunierbasabe26@gmail.com
tel: +55-453529 2113

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Graphene Transfer Process.

The method used for direct graphene transfer relied on a dry technique using the PDMS polymer. In the initial step of the transfer process, a portion of the PDMS polymer, Poly(dimethylsiloxane), was cut to cover the entire area of the CVD graphene sample. Subsequently, the graphene sample was positioned within the PDMS, and once positioned, the CVD graphene was pressed against the PDMS. Following this, the sample was sandwiched between the two glass plates, with a 10 kg lead block placed atop the plates to apply pressure and facilitate the transfer of graphene to the PDMS. The samples were subjected to the pressure of the lead block for 12 hours.

In the initial phase of the second stage, upon removal of the weight from the samples, graphene was removed from the portion not in contact with the PDMS polymer to prevent the transfer of two layers of graphene to the target substrate. This involved a mechanical removal of graphene followed by treatment with HNO3 in an aqueous solution, in a ratio of 3 parts HNO_3 to 1 part Milli-Q Water (3 mL of HNO_3 and 9 mL of Milli-Q Water). The surface of the copper not in contact with the PDMS was immersed in the solution for 5 minutes to ensure complete removal of the graphene from the other side.

The third step of the process involved the corrosion of copper using an Ammonium Persulfate solution (NH4)2 S2 O8 LabSynth lot 207015, at a concentration of 1.2 mol/L. After preparing the solution, the samples with PDMS, copper, and graphene were positioned with the copper side facing the solution. Following the complete corrosion of the copper, the solution was rinsed to remove the copper ions, and the samples, now comprising PDMS and graphene, were washed with Mili-Q water and dried with nitrogen for the subsequent step. Once dried, the graphene was ready for transfer to the target substrate. This involved affixing the PDMS with graphene onto the SiO_2 substrate, which had been cleaned with Isopropyl Alcohol and Acetone, each for 10 minutes in an ultrasonic bath operating at a frequency of 40KHz.

Following the application of the weight, graphene was successfully transferred from the PDMS to the SiO_2 substrate, requiring only the complete removal of the polymer from the substrate to finalize the transfer process.

This method is free of polymeric residues as it involves mechanically removing the 0.5 mm PDMS sheet using tweezers without the need for organic solvents.

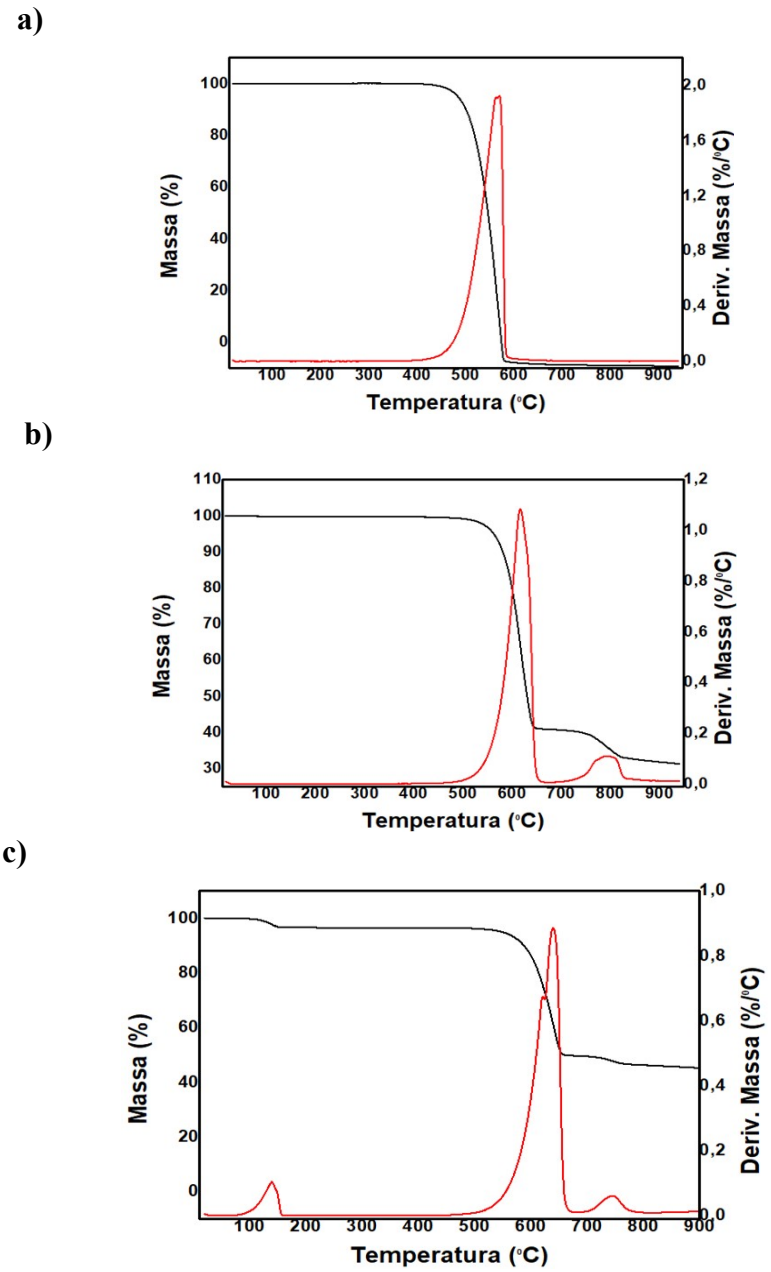

Fig. SI1 Thermograms curves of phthalocyanine molecules a) Pc4 (free metal), b) CoPc (Cobalt central atom), and c) CuPc (Cupper central atom).

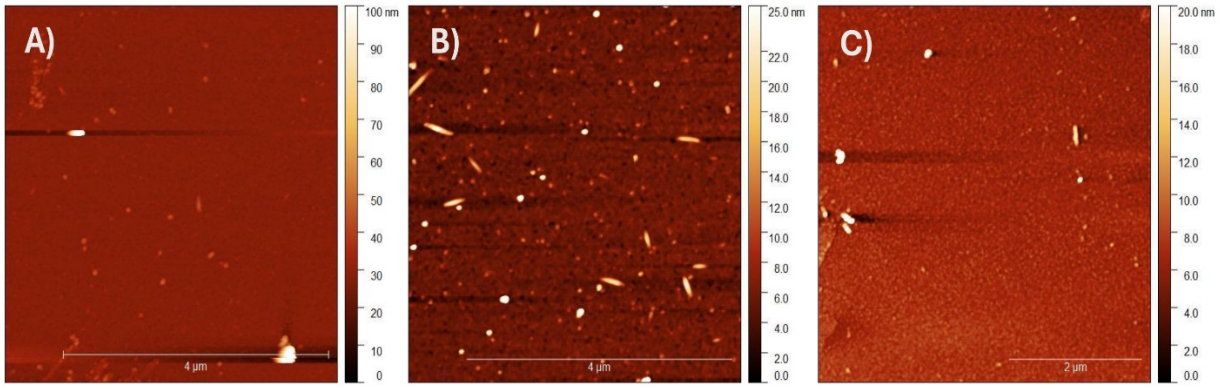

Fig. SI2. AFM images of the a) Pc4, b) CoPc and c) CuPc molecules deposited on graphene/SiO_2/Si substrate.

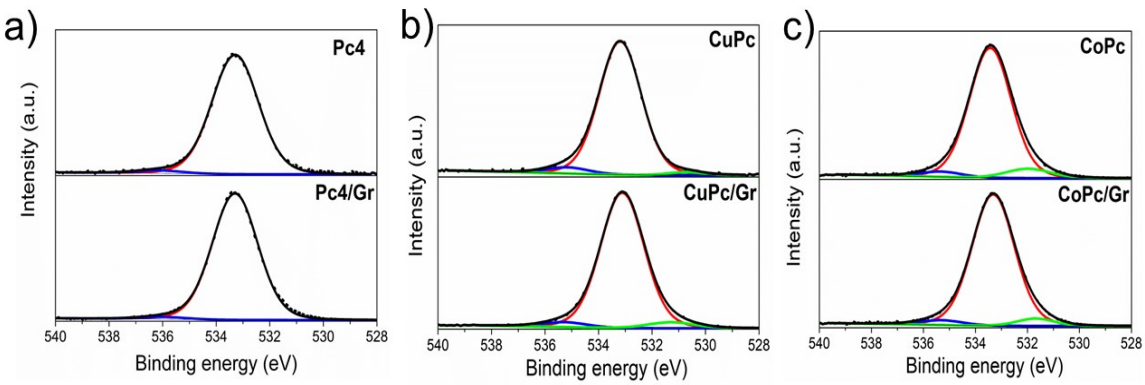

Fig. SI3. O 1s XPS spectra of the phthalocyanine molecules MePc deposited on SiO_2/Si wafer (upper panel) and on graphene (Gr, lower panel). a) Pc4, b) CuPc, and c) CoPc molecules