Electronic Suplementary Information to

A Hybrid Material Assembled by Anthocyanins from Açaí Fruit Intercalated between niobium lamellar oxide

Ângela Albuquerque Teixeira-Neto[a], Ana Lucia Shiguihara[a], Celly M. S. Izumi[a], Marcos Augusto Bizeto[b], Fabrice Leroux[c], Marcia L. Arruda Temperini[a] and Vera R. Leopoldo Constantino*[a]

[a] *Instituto de Química, Universidade de São Paulo, Av. Prof. Lineu Prestes 748, CEP 05508-000, São Paulo-SP, Brazil.*

[b] *Departamento de Ciências Exatas e da Terra, Universidade Federal de São Paulo - Campus Diadema, Rua Prof. Artur Riedel, 275, CEP 09972-270, Diadema-SP, Brazil.*

[c] *Laboratoire des Matériaux Inorganiques, UMR CNRS 6002, Université Blaise Pascal, 24, avenue des Landais, 63177 Aubière Cedex, France.*

Cyanidin-3-glucoside molecule possesses dimensions of 12 x 6.3 x 12 Å (Fig. S1) when in its most stable configuration (simulation carried on with the aid of Chem3D software, from CambridgeSoft Corp., using MM2 method).

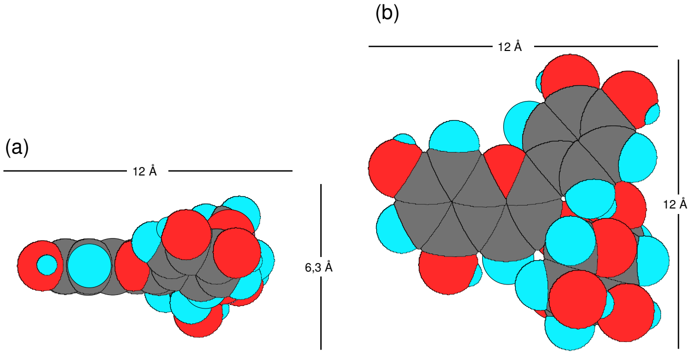

Fig. S1. Space-filling models of the cyanidin-3-glucoside molecule in its most stable configuration.

Fig. S2 shows pictures of dye-hex$_{exf}$ 80mL/g sample before and after heating process at 170^{o}C under air atmosfere in the TG-DSC furnace (Netzsch thermoanalyser model TG/DSC 490 PC Luxx). No color changes were observed.

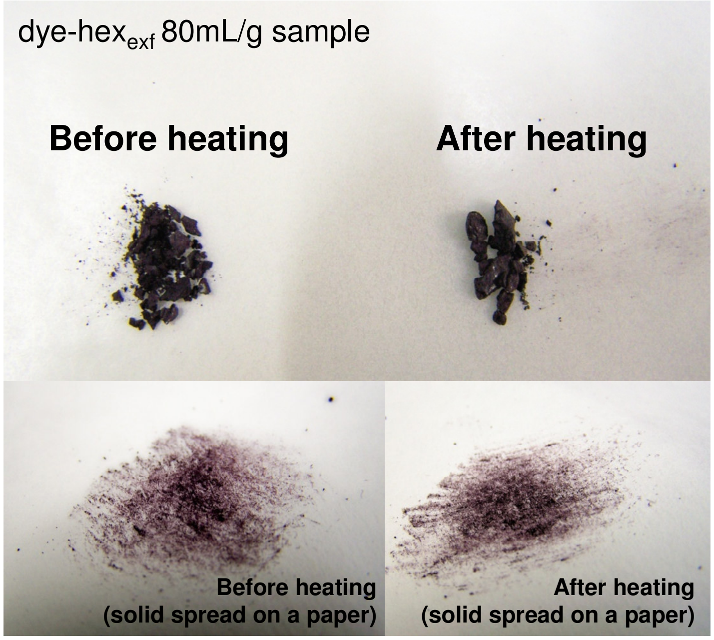

Fig. S2. Pictures of dye-hex$_{exf}$ 80mL/g sample before (left) and after (right) heating process at 170^{o}C under air.

Fourier transform infrared spectra (FTIR) were recorded on a Bomem spectrophotometer, model MB-102, with a reflectance accessory; the samples were diluted in solid KBr. FTIR spectra of dye-hexaniobate samples are presented in Fig. S3. The spectra of both dye-hex$_{exf}$ sample (Fig. S3a) and dye-hex$_{int}$ material (Fig. S3b) are very similar, although the spectra of their precursors are very different between them.

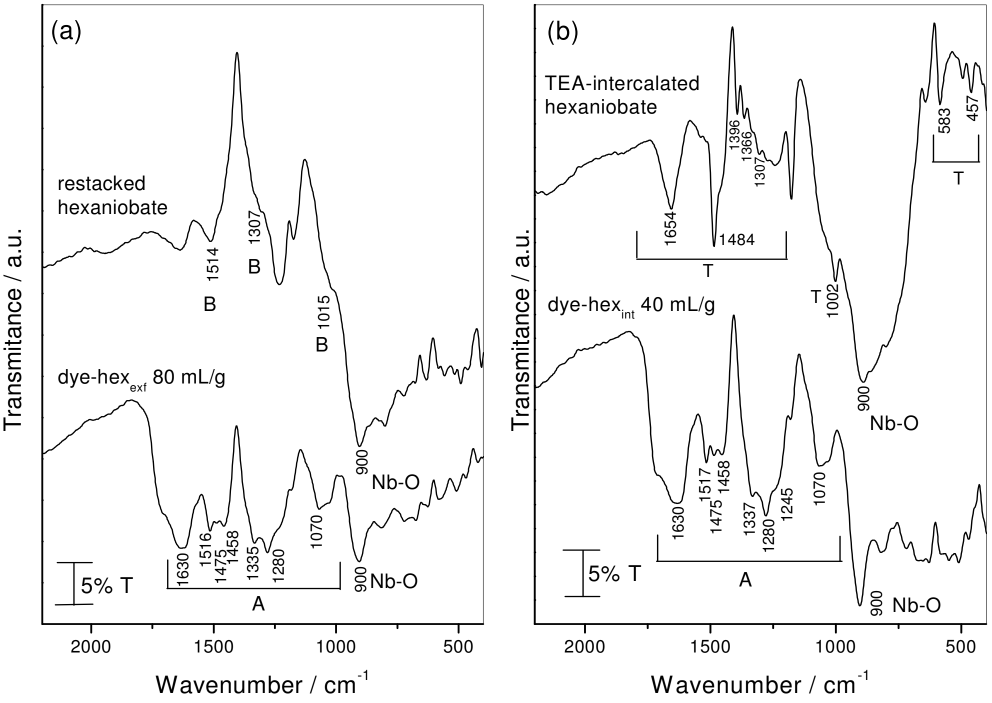

Fig. S3. FTIR spectra of (a) dye-hex$_{exf}$ sample and (b) dye-hex$_{int}$ sample. For comparison purposes, FTIR spectra of their respective precursors are also shown

The bands at about 1070 cm^{-1} (δ_{C-H}), 1245 and 1280 cm^{-1} (ν_{C-O} from phenols), 1335 cm^{-1} ($\nu_{C-C\ inter-ring}$), 1458, 1475, 1516 and 1630 cm^{-1} (ν_{C-C} from ring stretching) are due to anthocyanin group (marked with A) and are in agreement to the FTIR spectra of some hydroxyflavylium derivatives previously reported.[1] FTIR spectra of hybrid samples also show absorption bands that can be correlated to sugar units such as glucose.[2] The absorption band at 900 cm^{-1} (ν_{Nb-O}) and in the 500-700 cm^{-1} range are assigned to the inorganic phase.[3,4] Bands marked with B and T are due to n-butylamine or TEA$^+$ cations in the precursors samples respectively (Fig. S3).

Field emission scanning electron microscopy (FEG-SEM) images of carbon coated samples were obtained in a JEOL microscope, model JSM-7000F, at the Instituto de Química (Universidade de São Paulo - USP). FEG-SEM images of dye-hexaniobate hybrids (Fig. S4) reveal the presence of platelets in a face-to-face array in both dye-hex$_{exf}$ (Fig. S4a) and dye-hex$_{int}$ (Fig. S4b) samples. This kind of morphology corroborates the supposition that exfoliated hexaniobate layers are restacked when in presence of the cation dye, leading to a face-to-face oriented layered material with morphology similar to that observed for dye-hex$_{int}$ sample.

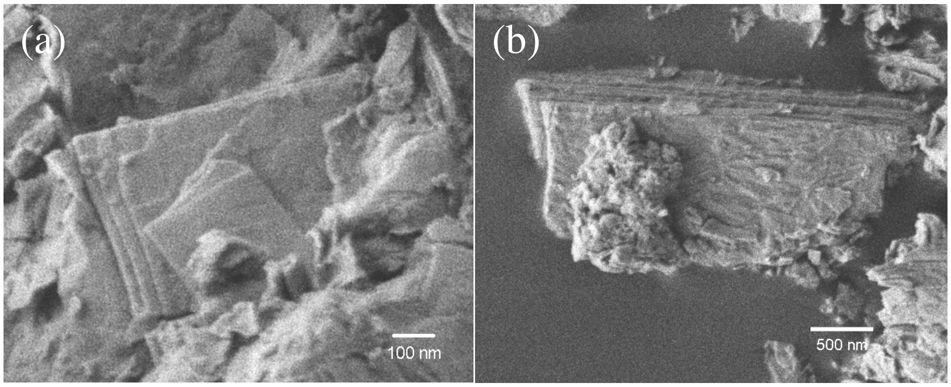

Fig. S4. SEM images of (a) dye-hex$_{exf}$ 80mL/g sample and (b) dye-hex$_{int}$ sample.

References

1. J.C. Merlin, J.P. Cornard, A. Stastoua and M. Saidi-Idrissi, *Spectrochim. Acta,* 1994, **50A**, 703.

2. M. Kacurakova and M. Mathlouthi, *Carbohydr. Res.,* 1996, **284**, 145.

3. J.M. Jehng and I.E. Wachs, *Chem. Mater.,* 1991, **3**, 100.

4. M.A. Bizeto, F.P. Christino, M.F.M. Tavares and V.R.L. Constantino, *Quim. Nova,* 2006, **29**, 1215.