Electronic Suplementary Information to

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

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

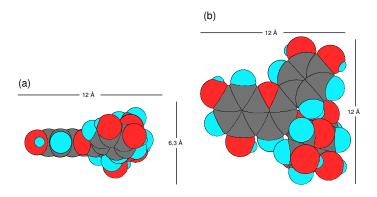


Fig. S1. Space-filling models of the cyanidin-3-glucoside molecule in its most stable configuration.

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

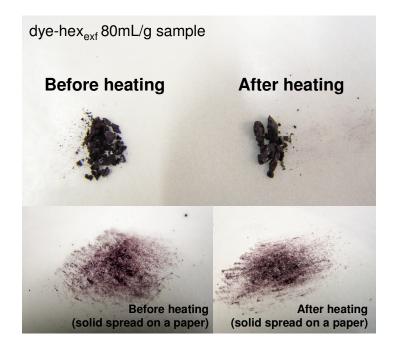


Fig. S2. Pictures of dye-hex_{exf} 80mL/g sample before (left) and after (right) heating process at 170°C under air.

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.

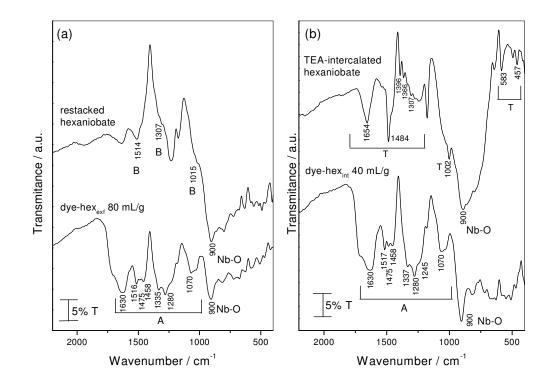


Fig. S3. FTIR spectra of (a) dye-hex_{exf} sample and (b) dye-hex_{int} sample. For comparison purposes, FTIR spectra of their respective precursors are also shown

The bands at about 1070 cm⁻¹ (δ_{C-H}), 1245 and 1280 cm⁻¹ (v_{C-O} from phenols), 1335 cm⁻¹ (v_{C-C} inter-ring), 1458, 1475, 1516 and 1630 cm⁻¹ (v_{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 (v_{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.

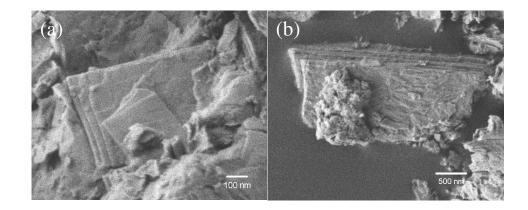


Fig. S4. SEM images of (a) dye-hex_{exf} 80mL/g sample and (b) dye-hex_{int} sample.

References

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