Improvement of NIR photophysical properties of a hemicyanine dye by its encapsulation within 1D-AIPO nanochannels

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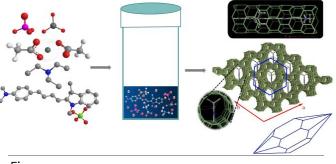
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Active fluorescent dyes based on small organic molecules in the near-infrared (NIR) region have awakened the interest for biomedical applications owing to minimize background interference and improve tissue depth penetration [1]. However, there are only a few dyes on the market representing this phenomenon. Thereupon, the design and synthesis of new advanced optic hybrid materials is currently a burning survey towards obtaining promising materials with enhanced properties [2]. In this work, the "one-pot" synthesis, based on the "in situ" encapsulation via crystallization inclusion method of the hemicyanine dye LDS 730 dye into 1D nanochannels of MgAPO-5 aluminophosphate, has led to a favourable bathochromic shift into the NIR spectra. The tight fitting between the molecular size of the guest dye and the pore dimensions of the host have enabled a rigid planar conformation of the Styril dye within the nanochannels [3]. Consequently, a boosted fluorescence in the NIR range of the spectra is enhanced during the occlusion with respect to the dye in solution together with alignment an among the channels. Therefore, a new hybrid material for the development of interesting potential optical properties and biomedical applications was achieved.

References

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[3] R. Sola-Llano, V. Martínez-Martínez, Y. Fujita, L. Gómez-Hortigüela, A. Alfayate, H. Uji-i, E. Fron, J. Pérez-Pariente, and I. López-Arbeloa, Chem. - A Eur. J (2016), vol. 22, 15700–15711.



Figures

Figure 1: Hydrothermal synthesis of the red emitting LDS 730/AFI hybrid materials via microwave. The dye is embedded and confined in the zeolite matrix during the crystal growth.

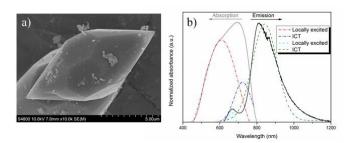


Figure 2: Molecular structure of the red-emitting LDS 730 dye with its respective dimensions calculated by optimizing the ground geometry using B3LYP hybrid functional (DFT) via Gaussian 09. B) The structure of AFI, MgAPO-5 aluminophosphate.

Imaginenano2018