Photoactive host-guest hybrid material for Non-Linear Optics by the encapsulation of LDS 722 dye into a 1-D nanochanneled aluminophosphate

Rebeca Sola-Llano[1], Virginia Martínez-Martínez[1], Yasuhiko Fujita[2], Luis Gómez-Hortigüela[3], Almudena Alfayate[3], Eduard Fron[2], Joaquín Pérez-Pariente[3], Iñigo López-Arbeloa[1]

[1] University of the Basque Country (UPV/EHU), Aptdo 644, 48080 Bilbao, Spain
[2]Katholieke Universiteit Leuven, Department of Chemistry, Celestijnenlaan 200F, B-3001 Heverlee, Belgium
[3]Catalysis and Petrochemistry Institute-CSIC, c/Marie Curie 2, 28049 Cantoblanco, Madrid, Spain

E-mail: rebeca.sola@ehu.eus

One approach to achieve photoactive hybrid materials with interesting properties for optical applications consists on the encapsulation of organic fluorophores into rigid inorganic frameworks. In this sense, it has been demonstrated that MgAPO-11, a magnesium aluminophosphate with AEL structure and 1-D nanochannels, is a suitable host to guest dyes with a general molecular structure built up by three fused aromatic rings since it prevents dye aggregation due to its tight pores (6.5 Å x 4 Å) with special topology, consisting on pockets, as shown in Fig. 1.[1,2] Also due to the narrow size of the nanochannels, the incorporation of the dyes should be carried out by crystallization inclusion method instead of by the typical post-synthetic approaches since diffusional processes are totally impeded.

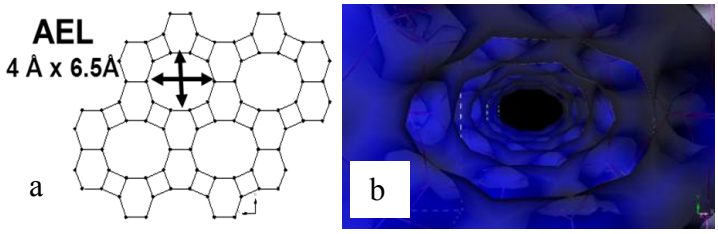

Figure 1. a) Structure and dimensions of the 1D-nanochannels of the AEL structure-type, b) Pore-topology of the same structure.

In order to find new nanostructured materials with applicability in the field of non-linear optics, a dye with intrinsic non-linear optical properties was chosen to be occluded into the MgAPO-11 matrix, the LDS 722. Although the synthesis of this type of dye-loaded MgAPOs is rather straightforward, an optimization of the synthetic procedure was required for the incorporation of this dye. Finally, the result was pure LDS722/AEL material which shows enhanced fluorescence capacity in comparison with the dye in solution (ϕ_{fl} (dye in aqueous solution) ~ 0.01 vs. ϕ_{fl} (LDS722/AEL) = 0.55). This is a direct consequence of the occlusion of such a flexible dye in a highly restricted and rigid environment that on the one hand, limits this flexibility, and on the other hand, forces the molecules to adopt a coplanar configuration (Fig. 2). Moreover, the hybrid material shows a highly anisotropic response to the linearly

polarized light due to the preferential alignment of the dyes within the tight pores. As a result, this material revealed attractive second-order non-linear properties such as Second Harmonic Generation (SHG) under NIR irradiation (Fig. 2), proven through microscopic techniques at single crystal level.[3]

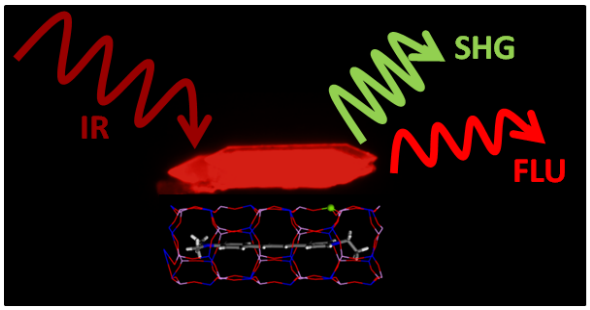

Figure 2. Fluorescence image of a LDS722/AEL crystal with an illustration of the processes arising under NIR illumination, together with a representation of the LDS 722 molecule within an AEL channel (down)

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