NanoSpain Conf 2017
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Development of nanostructured host-guest hybrid material for Non-Linear Optics

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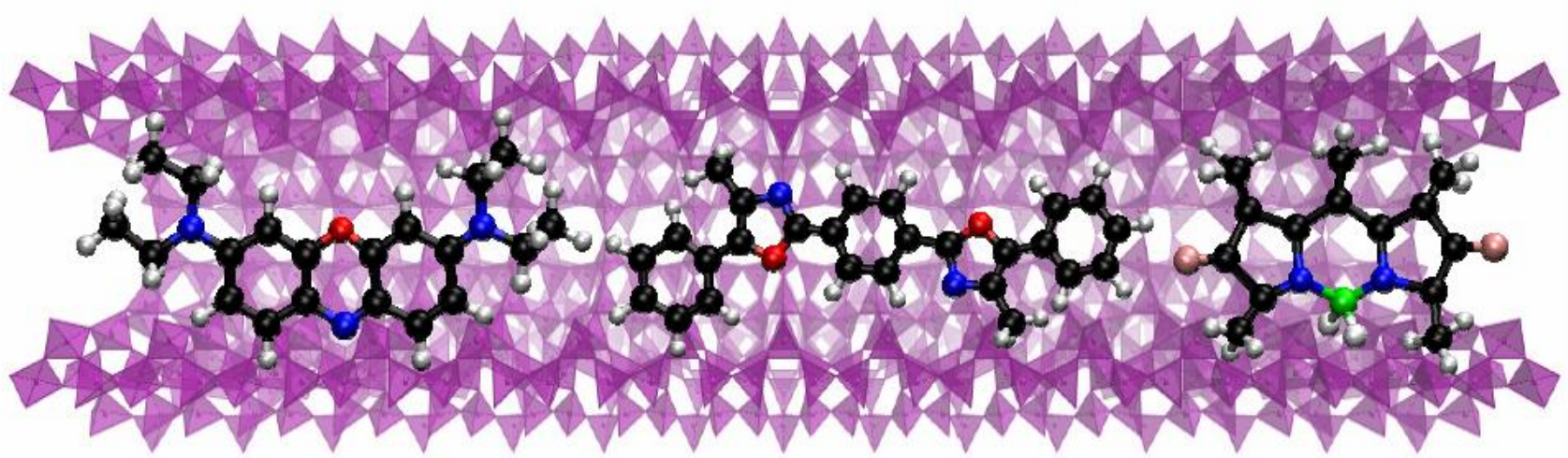
Occlusion Chemistry

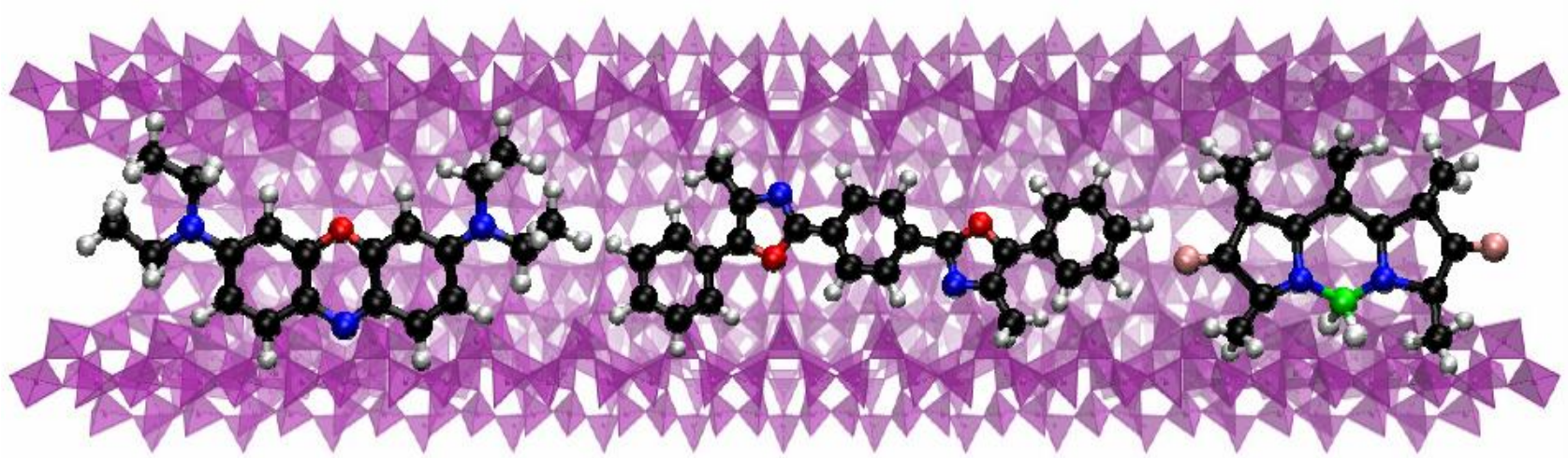


Supramolecular organization and improvement of the properties

↓

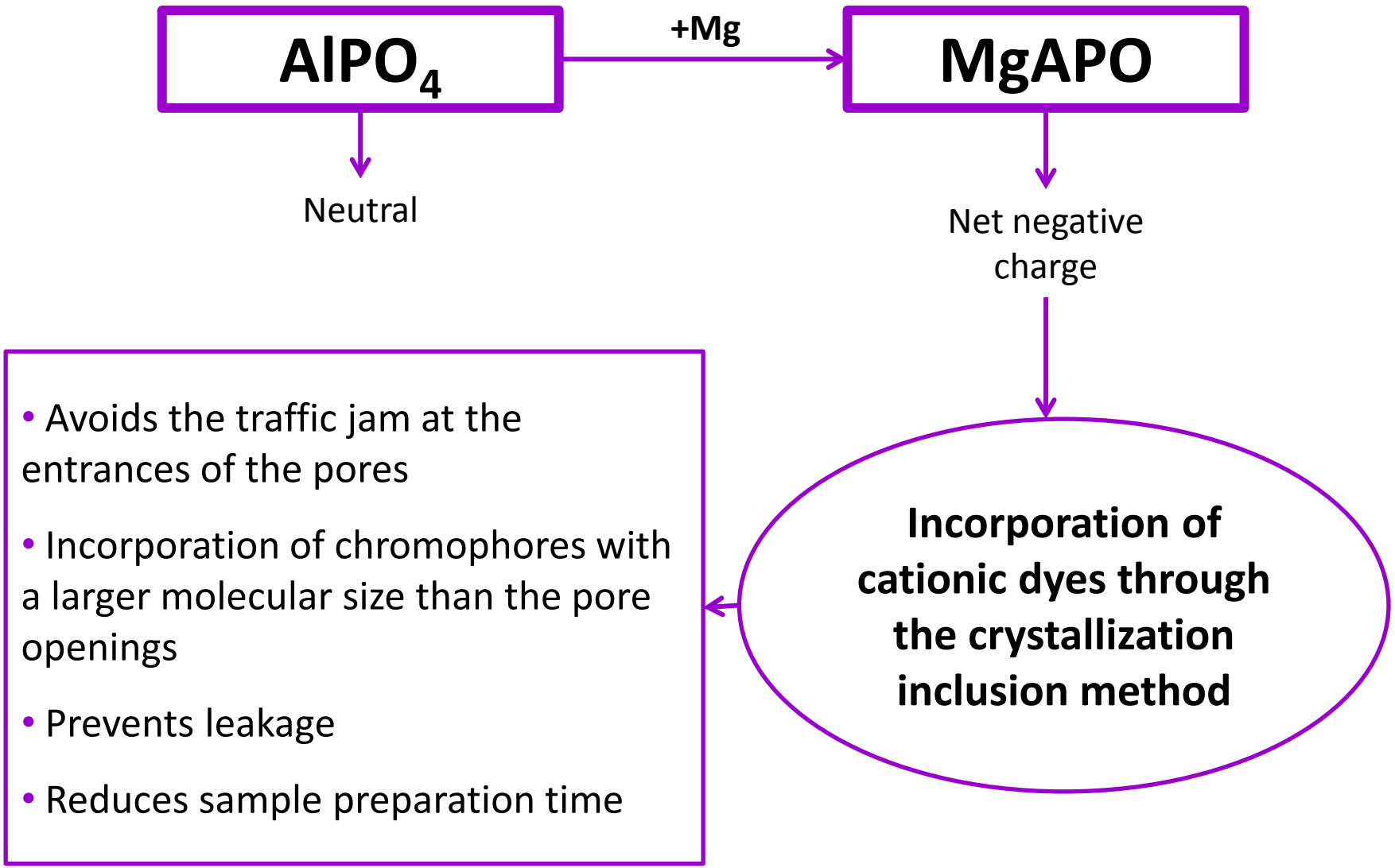
Anisotropic response → NLO

Occlusion Chemistry

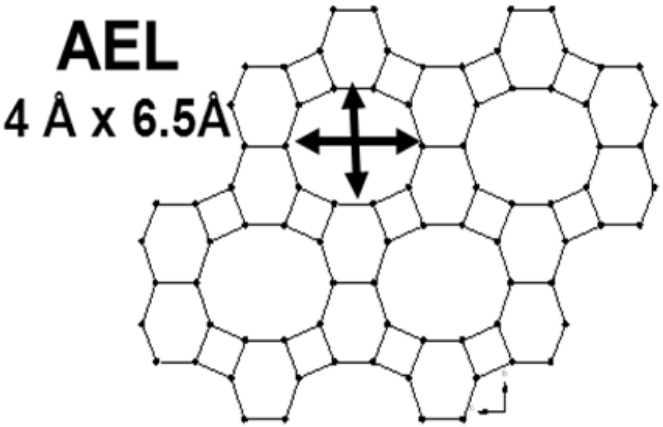


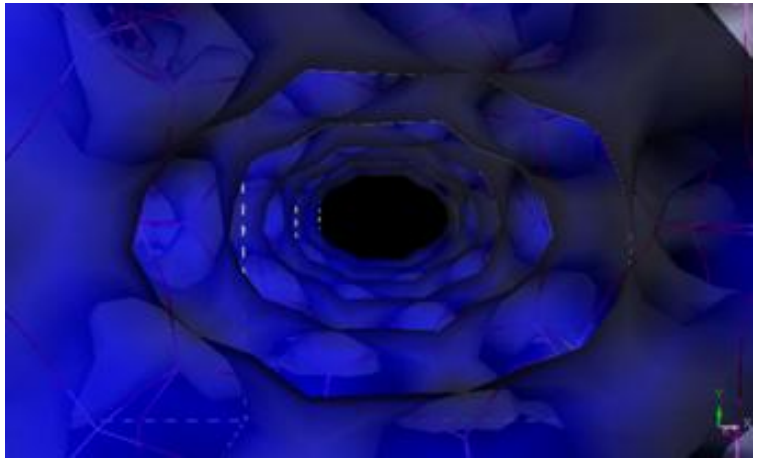
Optical applications

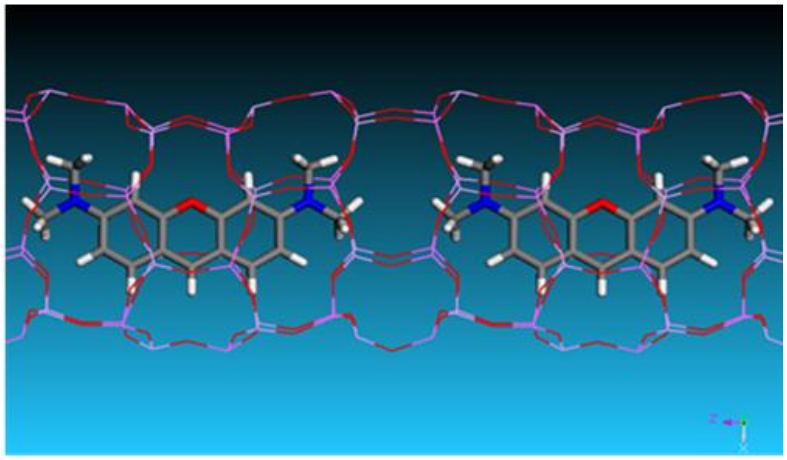
Optically dense materials → **Aggregation**


AlPO4
+Mg
MgAPO
Neutral
Net negative charge
Incorporation of cationic dyes through the crystallization inclusion method
• Avoids the traffic jam at the entrances of the pores
• Incorporation of chromophores with a larger molecular size than the pore openings
• Prevents leakage
• Reduces sample preparation time

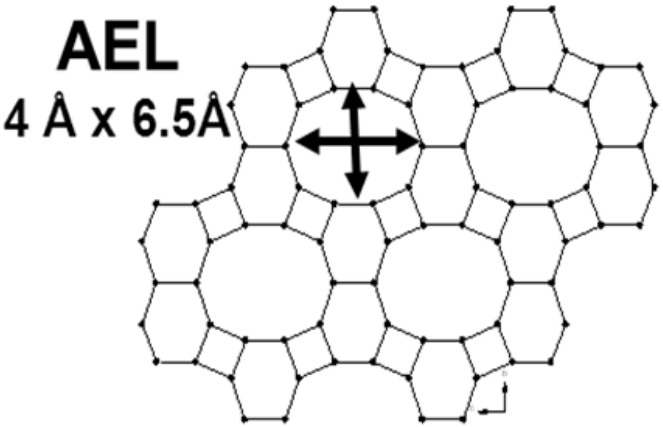
MgAPO-11

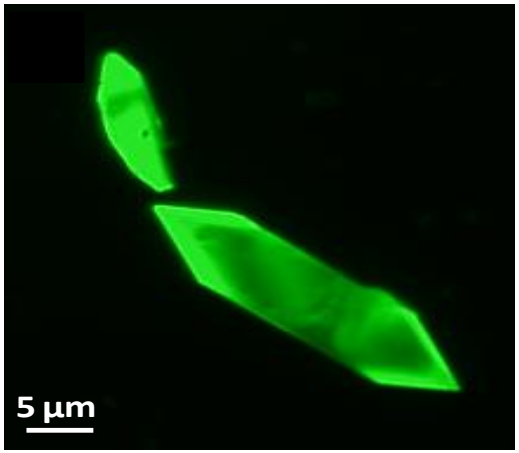


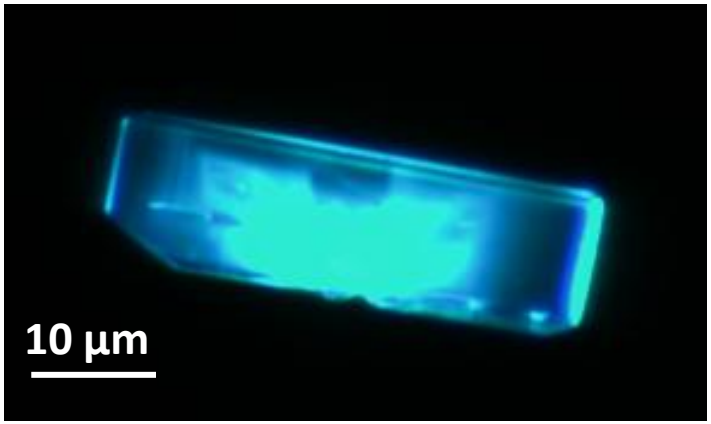




MgAPO-11







V. Martínez-Martínez, et al. *Chem.Eur.J.* **2013**, *19*, 9859.

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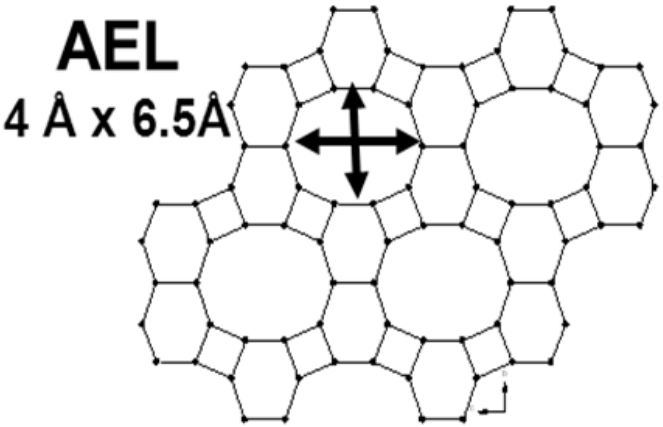
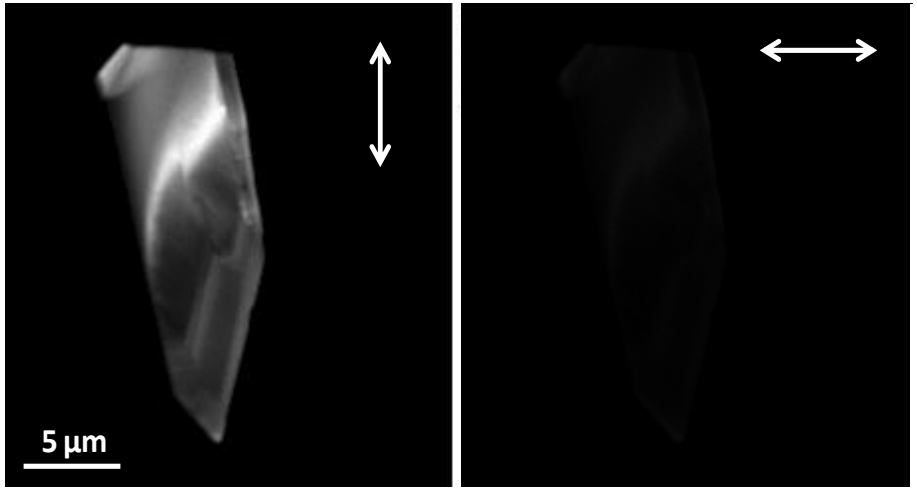
MgAPO-11





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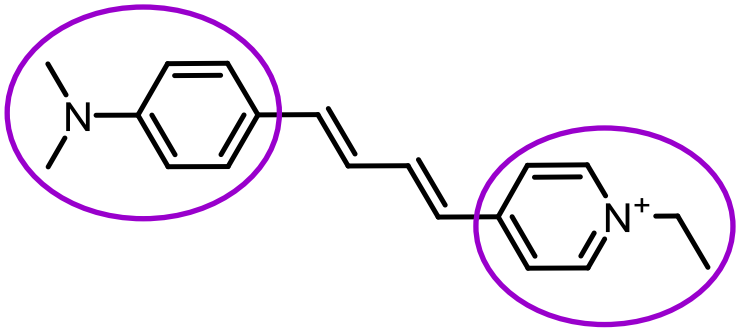
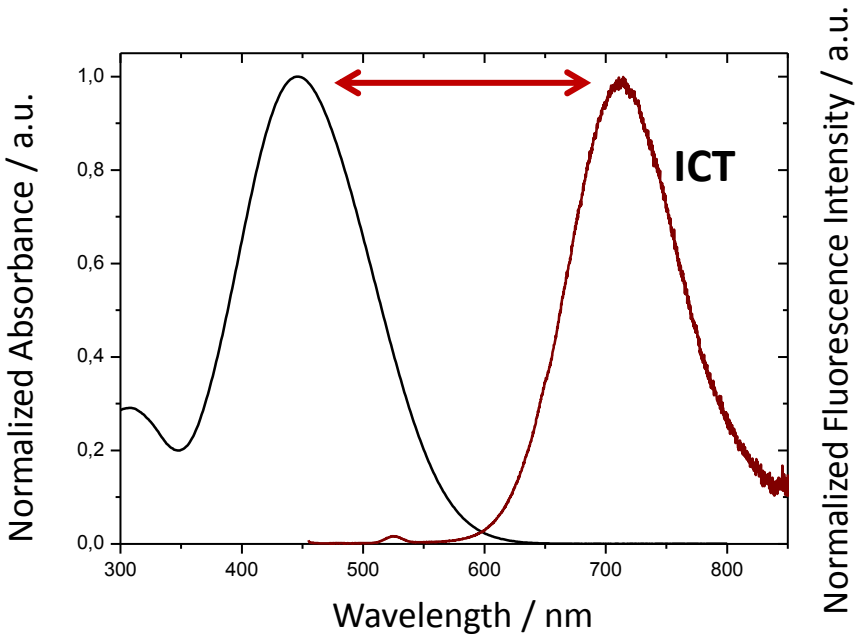
LDS722/AEL

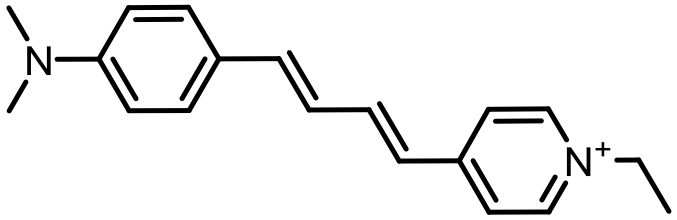


LDS 722

Minimize inner filter effects



LDS722/AEL



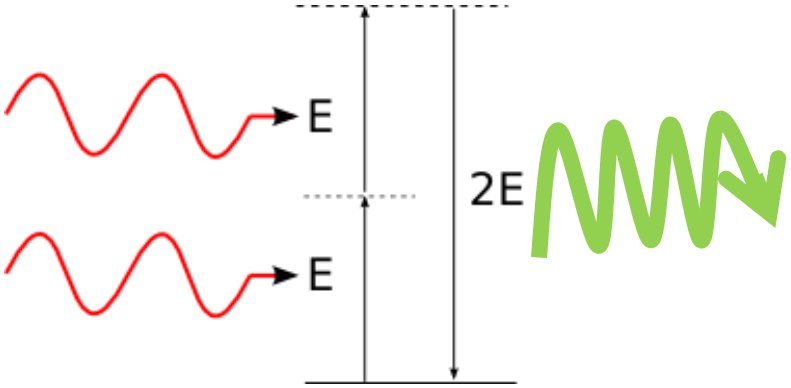
LDS 722

Change in the dipolar moment and high β values

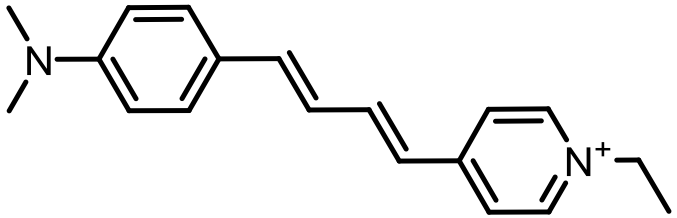
↓

NLO

SHG



LDS722/AEL



LDS 722

Change in the dipolar moment and high β values

↓

NLO

-Centrosymmetric crystallization

- Flexible molecules, fluorescence ↓

LDS722/AEL

Hydrothermal synthesis

Optimization of the synthesis procedure towards AEL phase

Systematic variation of:

i) Synthesis gel composition (Mg, EBA, dye content)
ii) Crystallization temperature and time
iii) Heating regime (static or dynamic)

LDS722/AEL

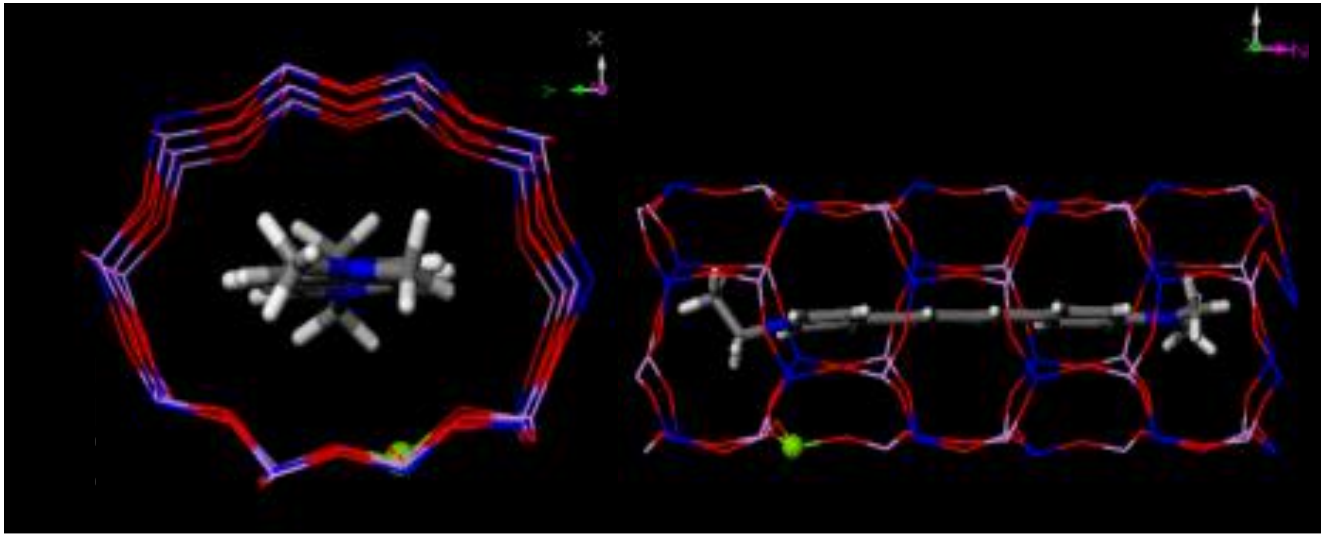
0.1 MgO : 1 P_2O_5 : 0.95 Al_2O_3 : 1 EBA : **0.008-0.024 LDS722** : 300 H_2O, carrying out the crystallization statically for 24 hours at 195ºC

R. Sola-Llano, et al. *Chem. – A Eur. J.* **2016**, *22*, 15700-15711.

LDS722/AEL

ϕ_{fl} (MgAPO-11/LDS 722) : **0.55**

ϕ_{fl} (LDS 722 aq.) : 0.01



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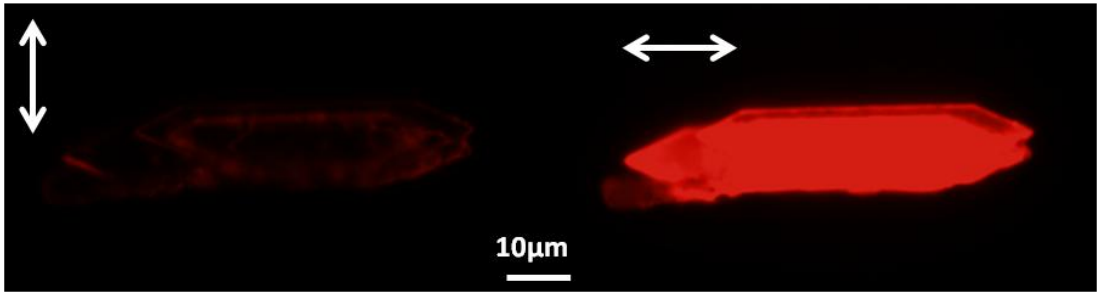

D ~ 50

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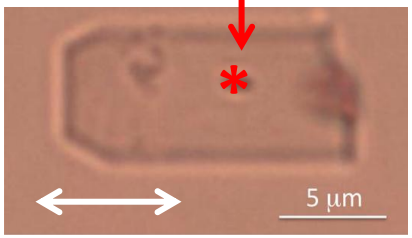
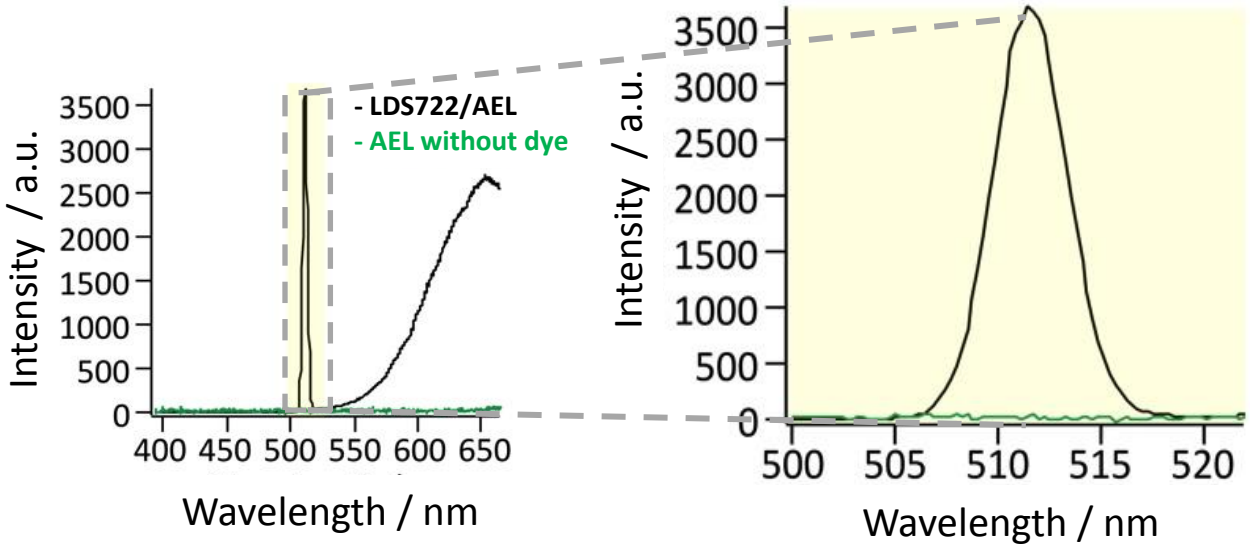
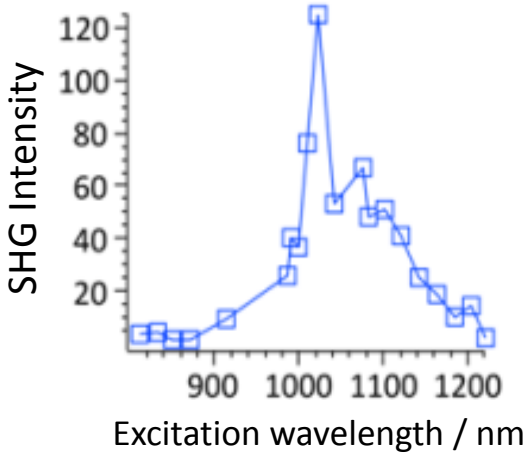
LDS722/AEL

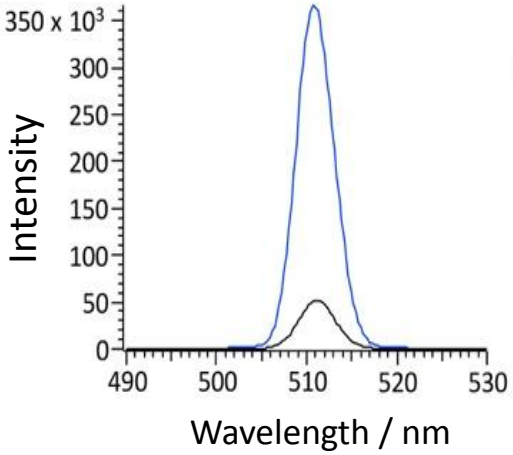
KU LEUVEN

λ_{exc} : 1024 nm









17%

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Conclusion

By the tight confinement of LDS 722 into MgAPO-11 (AEL structure) through the crystallization inclusion method:

- **Enhance fluorescence properties**
- **NLO properties**

Since

i) aggregation is prevented
ii) the flexibility of the molecules is limited and
iii) a preferential orientation of the encapsulated chromophores is achieved.

Acknowledgement

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- ❖ **Dr. Yasuhiko Fujita**
- ❖ **Dr. Eduard Fron**
- ❖ **Dr. Hiroshi Uji-i**

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