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## Non photochemical light induced nucléation

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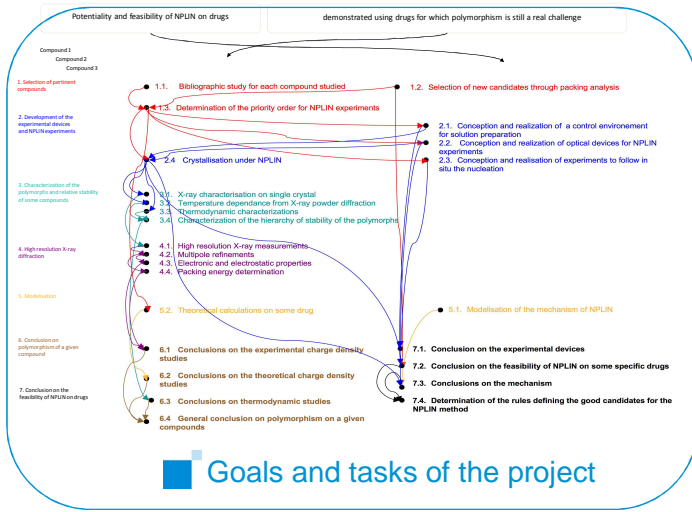
# NPLIN-4-drug

## Non Phototchemical Light Induced Nucleation for drugs

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### Journées Nationales en Nanosciences et Nanotechnologies 2012



**Polymorphism studies important in the industrial pharmaceutical context**

Method developed on urea [1], glycine [2], L-histidine [3], Hen Egg White Lysozyme [4], Bovine P T [5], Pentyl cyanobiphenyl [6], KCl [7] [9], NaClO<sub>3</sub> [8], KBr [9], Acetic acid [10]

[1] Garett B.A. et al. *Phys. Rev. Lett.* 1996,16, 3475-3476; Yoshikawa H.Y. et al. *Jpn J. Appl. Phys.* 2006, 45, 302-305; Yoshikawa H.Y. et al. *Jpn J. Appl. Phys.* 2006, 45, 1565-1567; Sun X.Y. et al. *Cryst. Growth Des.* 2005, 5, 684-689; Sugiyama T. et al. *Chem. Lett.* 2007, 136, 1489-1491; Sun X.Y. Ph.D. 2008; Sugiyama T. et al. *Chem. Lett.* 2009, 138, 482-483; [3] Sun X.Y. et al. *Cryst. Growth Des.* 2008, 8, 1720-1722; [4] Lee et al. *Crystal Growth & Design* vol.8 2008 n°12, 4255-4261 [5] Lee et al. *Crystal Growth & Design* vol.8 2008 n°12, 4255-4261 [6] Sun et al., *Phys. Rev. E* vol.79 2009 021701 [7] Alexander A.J. et al. *Cryst. Growth Des.* 2009, 9, 958-963; Duffus A.J. et al. *J. Am. Chem. Soc.* 2009, 131, 11676-11677; Ward M.R. et al. *Phys. Rev. Lett.* 2009, 481, 25-28. [8] Ward et al. *J. Chem. Phys.* Vol. 135 2011 114508 [9] Ward et al. *Crystal Growth & Design* vol.12 2012, 4554-4561 [10] Ward et al. *Phys. Chem. Chem. Phys.* 2011 Vol.14

**Context**

$$N(\alpha_{\text{parallèle}} - \alpha_{\text{perpendiculaire}})^2 = 45\epsilon_0 n_0 K_b T$$

- Co-existence of clusters of polarisability tensors of different symmetry: « disk-like » or « rod-like »
- Role of the induced dipolar moment depending on the clusters type
- Dipole moment induced of the cluster aligned itself on the laser polarization. Minimization of energy.

**Possible mechanism : Kerr effect**

**Electrostatic properties of piracetam and carbamazepine and phase diagram for piracetam (tasks 3.1, 3.3, 4.1, 4.3, 4.4)**

**Carbamazepine (task 2.4)**

**NPLIN new experimental device (task 2.1, 2.2, 2.3)**

A full automated NPLIN experiment with real time monitoring using Labview

**Conclusions and apertures**

- The device allows us to expose and survey till 90 samples during several days and it is fully automated.
- In a near future, the device will permit to study solubility according to temperature and to determine metastable zone.
- This device can probe a huge number of solutions using NPLIN method.
- Interesting results come from Carbamazepine, Glycine and glutamic acid.

### Production scientifique (publications, brevets)

- B. CLAIR, A. IKNI, H. YANG, F. DUMAS, P. SCOUFFLAIRE, A. SPASOJEVIC – DE BIRÉ « Non Photochemical Light Induced Nucleation. A tool to crystallize polymorphs on demand ? » CPOSS meeting, London (UK), Grande-Bretagne, 30 mars 2011
- A. IKNI, B. CLAIR, H. YANG, F. DUMAS, P. SCOUFFLAIRE, A. SPASOJEVIC – DE BIRÉ « Non Photochemical Light Induced Nucleation. A tool to crystallize polymorphs on demand ? » IV congrès algérien de cristallographie, Kenchela, (Algérie), 14-16 mai 2011
- A. SPASOJEVIC – DE BIRÉ, A. IKNI, B. CLAIR, N. GUILBIN, I. KORNEV, X. SHI, J. LONG, H. YANG, W. LI, M. MENDRE, P. SCOUFFLAIRE, E. JEAN-BART, J. BEAUNIER, F. SAIG, P. ESPEAU, Y. CORVIS, C. ALZINA, N-E GHERMANI, N. EL HASSAN, F. DUMAS, S. VEESLER, Z. HAMMADI « Non Photochemical Light Induced Nucleation » Journées nationales en nanosciences et nanotechnologies, Strasbourg (France) 7 – 9 novembre 2011
- A. SPASOJEVIC – DE BIRÉ, A. IKNI, B. CLAIR, F. DUMAS, P. SCOUFFLAIRE, « Non Photochemical Light Induced Nucleation (NPLIN). A tool to crystallize polymorphs on demand ? Application to carbamazepine » GFCC-2011, Paris, novembre 2011
- B. CLAIR, A. IKNI, P. SCOUFFLAIRE, S. VEESLER, A. SPASOJEVIC – DE BIRÉ « A Method to probe NPLIN on glycine and histidine : a new path to understand nucleation » CPOSS meeting, London (UK), 3 avril 2012
- A. IKNI, B. CLAIR, P. SCOUFFLAIRE, S. VEESLER, A. SPASOJEVIC – DE BIRÉ, « Non Photochemical Light Induced Nucleation (NPLIN). Application to carbamazepine (CBZ) » CPOSS meeting, London (UK), 3 avril 2012
- A. SPASOJEVIC – DE BIRÉ, P. SCOUFFLAIRE, A. IKNI, B. CLAIR, E. JEAN-BART, J. BEAUNIER, F. SAIG « New automated experimental devices for Non Photochemical Light Induced Nucleation » CPOSS meeting, London (UK), 3 avril 2012
- B. CLAIR, A. IKNI, P. SCOUFFLAIRE, A. SPASOJEVIC – DE BIRÉ, « NPLIN of glycine and carbamazepine » Serbian Crystallographic Meeting, Bela Crkva (Serbie), 31 mai – 2 juin 2012
- A. IKNI, B. CLAIR, P. SCOUFFLAIRE, A. SPASOJEVIC – DE BIRÉ, « NonPhotochemical Light Induced Nucleation of Carbamazepine in Polar protic and aprotic solvents » 2012 Collaborative Conference on Crystal Growth, Orlando (USA), 11-14 décembre 2012
- B. CLAIR, A. IKNI, P. SCOUFFLAIRE, A. SPASOJEVIC – DE BIRÉ, « Understanding photophysical effects : NPLIN on glycine and L- glutamic acid » 2012 Collaborative Conference on Crystal Growth, Orlando (USA), 11-14 décembre 2012

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