



ANR project: Nouveaux Outils pour la Simulation des Solides et des Interfaces

Partenaires:

- ✚ **CPMOH**, Bordeaux: D. Foerster, A. Marbeuf
- ✚ **LaBRI**, Bordeaux: M. Delest, D. Aubert, O. Coulaud, J.P. Domenger, A. Esnard, P. Mary
- ✚ **IPREM**, Pau: I. Baraille, P. Bordat, R. Brown, J.C. Dupin, H. Martinez

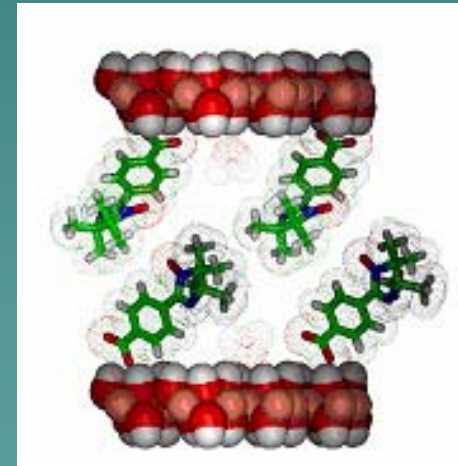
- ✚ **DRIMM**, Bordeaux: J. Bernard, N. N. Ky

- ✚ **Institut Néel**, Grenoble: E. Dooryhée, P. Martinetto

- ✚ **CCLRC**, Daresbury (England): P. Sherwood, W. Smith, I. Todorov
- ✚ **DIPC**, San-Sebastian (Spain): D. Sanchez, J. Junquera, P. Orderon, J. Soler

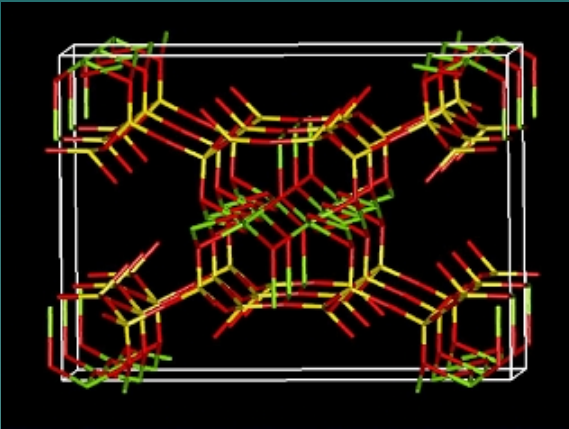
Aim: Understanding of the connection between structure and properties at the mesoscopic scale of hybrid organic-inorganic materials

- ↳ Complex and costly design of new materials
- ↳ Wide contribution of computer simulations
- BUT:** absence of some crucial functions
- ↳ **Development of new tools** for simulation of hybrid materials (inorganic crystalline or amorphous host in which dyes are encapsulated or grafted)
- ↳ **New functional materials** with diversified and flexible properties
 - ✚ Biotechnologies, medicine (diagnosis and therapy)
 - ✚ Nontoxic coatings (paint pigment)
 - ✚ Energy (photovoltaic cell)
 - ✚ Depollution of air or water (photo-catalytic materials)
 - ✚ Optoelectronic devices

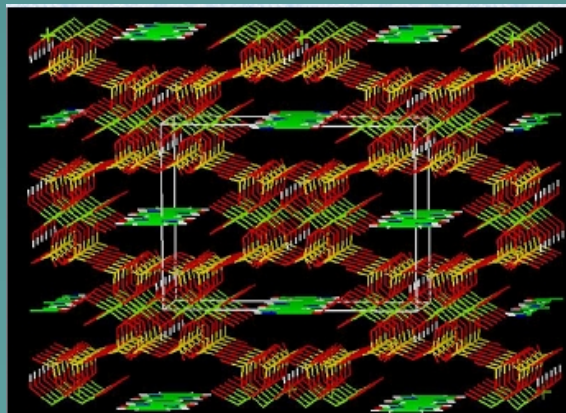


Example: Maya blue (Collaboration IPREM/Institut Néel)

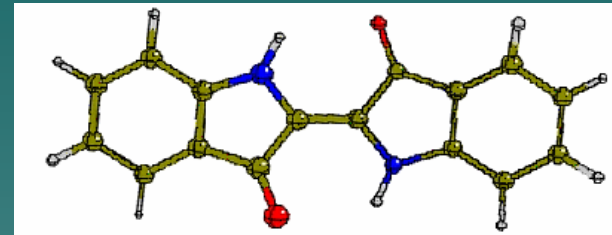
Palygorskite $(\text{MgAl})_2\text{Si}_4\text{O}_{10}(\text{OH})_2 \cdot 4\text{H}_2\text{O}$





Thermic and mechanic stabilities



Indigo



Blue colour resists to
 time
 nitric acid attack

 Where is indigo?
 How is indigo protected?

Hybrid organic-inorganic materials

Transition energy calculation :

$$\Delta\varepsilon = \Delta\varepsilon(\text{intra}) + \Delta\varepsilon(\text{inter})$$

Isolated organic molecule
Quantum-mechanical methods
(QM)

↪ DFT

↪ TDDFT

Environment (inorganic host material)

Classical molecular dynamics

↪ Parameterization of empirical potentials

Coupling QM/MD

Visualization, steering

Parallel codes
(MD: DLPOLY, QM: SIESTA)

Experimental validation (Absorption,
fluorescence spectroscopy and
microscopy, DRX, XPS)

NOSSI organization and means

		Year 1	Year 2	Year 3
PART A: QM/MM coupling	A1 DFT/MM coupling (ECP/LaBRI/CPMOH)	PhD	Post-doc A2 (ECP/LaBRI)	
	A2 Development TDDFT(C PMOH/ECP)	Post-doc A1 ECP/CPMOH	PhD	
	A3 TDDFT/MM coupling (ECP/ LaBRI/CPMOH)			PhD
	A4 Applications of the TDDFT/MM code (ECP/CPMOH/SPM-CE)			post-doc A2 (ECP/LaBRI)
				post-doc A3 (ECP/SPM-CE)
PART B : Empirical potentials	B1 Systematic errors (SiO ₂)	Post-doc B1 (ECP/CPMOH)		
	B2 Empirical potentials		Post-doc B2 ECP/ CPMOH	
PART C : Graphical and steering tools	C1 Redistribution scheme	Application to DL_POLY	Application to the DFT/MM code	Application to the TDDFT/MM code
	C2 Data interdependence			
	C3 Data mining	Engineer LaBRI/DRIMM		
	C4 Graphics placement			