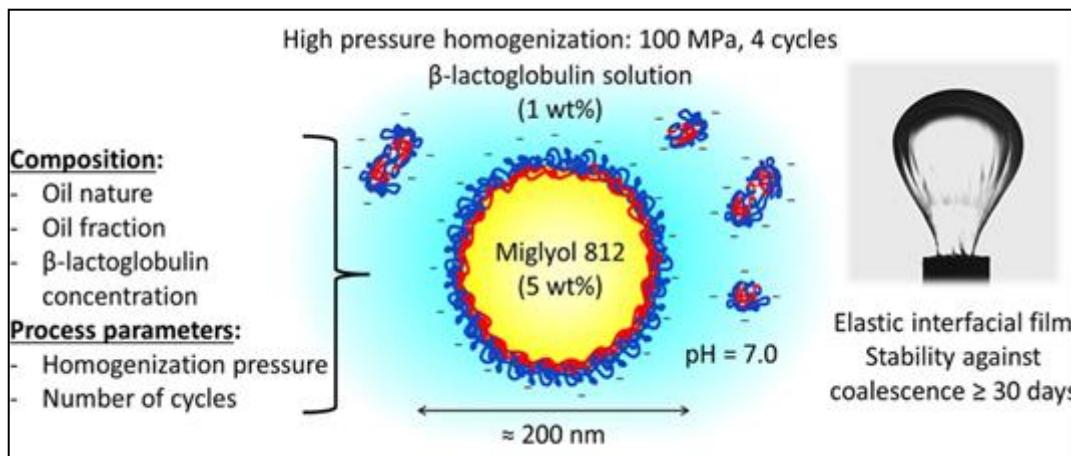
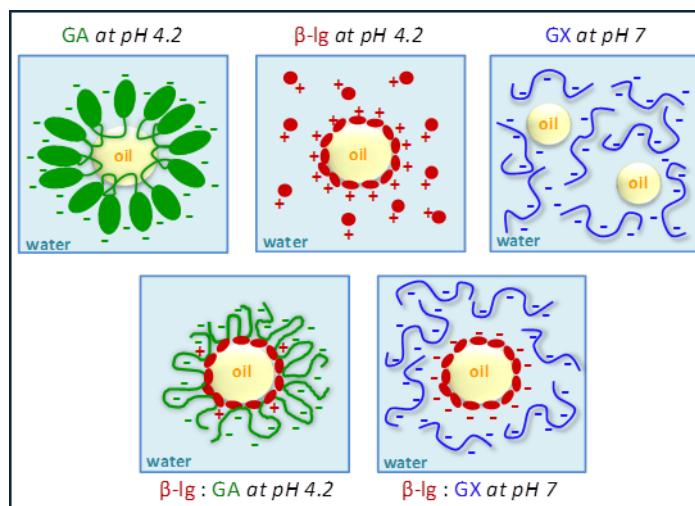


Publications majeures de l'équipe 3

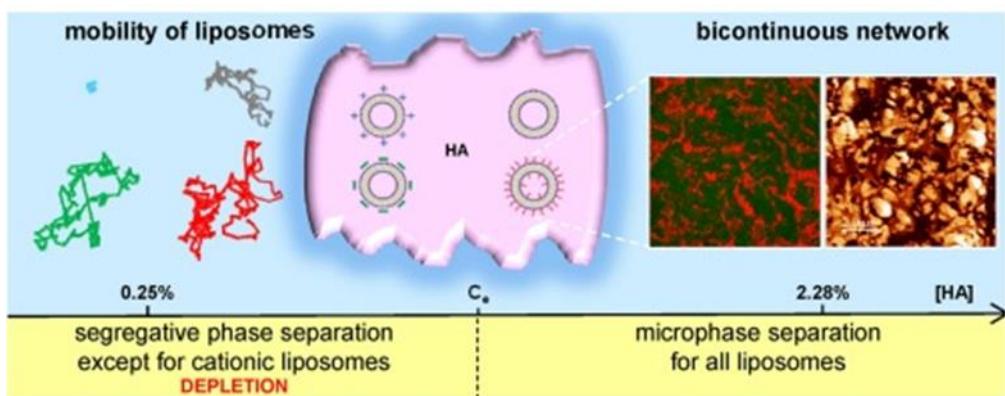
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Experimental electron densities of neutral and zwitterionic forms of piroxicam drug

Received 00th January 20xx,
Accepted 00th January 20xx

DOI: 10.1039/x0xx00000x

www.rsc.org/

The electron and electrostatic properties of piroxicam (PX) were derived from high resolution X-ray diffraction experiments carried out at 100 K. Two forms of the piroxicam molecule have been investigated in their crystalline states. One molecule is neutral (nPX) in form I (monoclinic) of piroxicam, while the second found in the hydrated pseudopolymer (triclinic) is zwitterionic (zPX). In the zPX crystal, the asymmetric unit is formed by two PX molecules with different conformations. The experimental electron density was refined using the Hansen-Coppens multipole model. The electron densities were carefully analyzed using the Atoms in Molecules approach of Richard Bader. Integrated atomic charges compare well for the nPX and zPX molecules. The negative electrostatic potential is found more extended for the zPX molecules than in the nPX one, probably due to the presence of the water molecules connected via hydrogen bonds. The electrostatic potential values on the molecular surface (isodensity of 0.007 e \AA^{-3}) were statistically analyzed in order to reveal local polarity, variances of the positive and negative regions, charge separation etc. In the nPX crystal, the molecular dipole is found equal to 9.12 D with a local dipole of 9.28 D for the SO₂CN fragment. The two molecules in the asymmetric unit of the zPX crystal display dipole moment magnitudes respectively equal to 6.83 D and 22.69 D; the corresponding SO₂CN sulfonyl cyanide fragment dipoles are 10.88 D and 13.64 D. Comparisons were made for the same fragment in the sulfathiazole molecule. Hence, we have also studied the polymorphs III and IV of the sulfathiazole; the asymmetric unit for polymorph III contains two molecules. The resulted SO₂CN dipole moment values are 11.19 D and 11.18 D found for the two molecules in polymorph III and 12.34 D for polymorph IV of the sulfathiazole. The intermolecular electrostatic interaction and the empirical packing energies are estimated to characterize the crystal packing of the two forms of piroxicam.

Xiao Xu, Anne Spasojević-de Biré, Nour Eddine Ghermani, Yongge Wei, Sladjana Novaković, Nada Bošnjaković-Pavlović and Pingfan Wu. Experimental evidence of charge transfer in a functionalized hexavanadate: a high resolution X-ray diffraction study. *Phys. Chem. Chem. Phys.*, **2017**, *19*, 18162–18166. DOI: 10.1039/C7CP01840A.



Cite this: *Phys. Chem. Chem. Phys.*, 2017, *19*, 18162

Received 22nd March 2017,
Accepted 15th June 2017

DOI: 10.1039/c7cp01840a

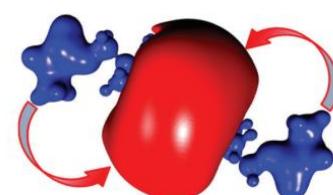
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Experimental evidence of charge transfer in a functionalized hexavanadate: a high resolution X-ray diffraction study†

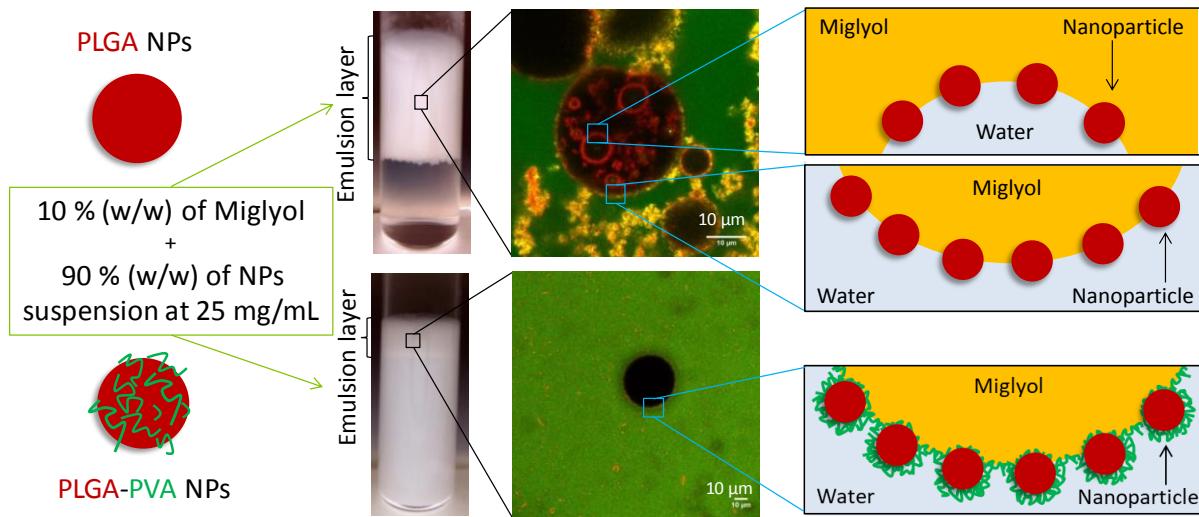
Xiao Xu,^{a,b} Anne Spasojević-de Biré,^{b,*ab} Nour Eddine Ghermani,^{abc} Yongge Wei,^d Sladjana Novaković,^{a,e} Nada Bošnjaković-Pavlović^{a,f} and Pingfan Wu^g

A high resolution X-ray diffraction study has been carried out on $[(\text{C}_6\text{H}_5)_2\text{N}]_2[\text{V}_6\text{O}_{13}\{(\text{OCH}_2)_5\text{CCH}_2\text{OCCH}_2\text{CH}_3\}_2]$ (V6–C3) at 100 K. The V6 core possesses a negative charge, leading to a strong polarization of the anion. A nucleophilic region localized near the organic moiety and an electrophilic region in the vicinity of the V6 core provide an overall description of charge-transfer behavior.

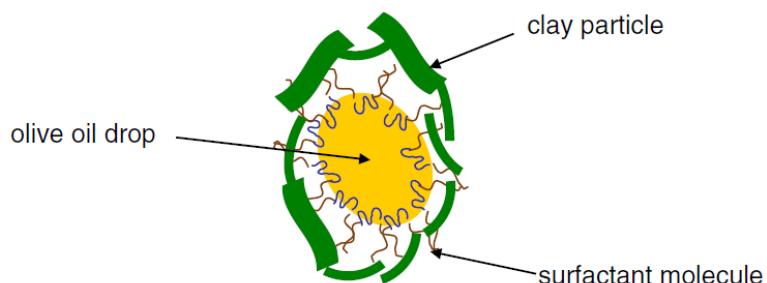
CT materials containing the spherical POM acceptors (Lindqvist-type $[\text{Mo}_8\text{O}_{19}]^{2-}$ and Keggin-type $[\text{SiMo}_{12}\text{O}_{40}]^{3-}$) and planar arene donors exhibit unique structures and potential nonlinear optical and ferromagnetic properties.⁹ TTF-POM CT materials (TTF means tetraphiafulvalene) show semiconductor properties and have potential application in semiconductor devices.^{8b,10}



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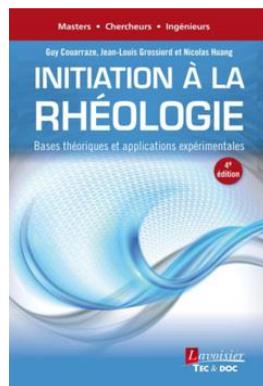
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Model of clay particles and surfactant molecules distribution in oil-in-water emulsions:
formation of a particles sublayer

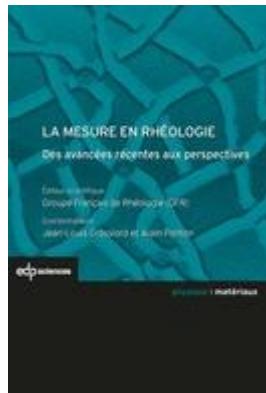
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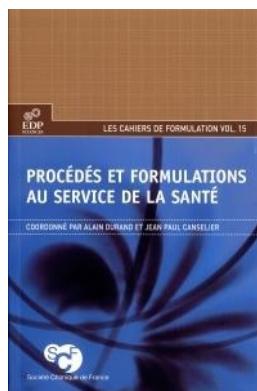


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