Liquid Crystal Nanocomposites for Photovoltaics: Using what we have or will learn to look at the Influence of Structure in Modeling the Transport of Electrons

L. J. Martínez-Miranda
University of Maryland
Dept of Materials Science and Eng.
University of Maryland Energy Center
College Park, MD
CUWIP – 18 January 2015

Liquid Crystal Nanocomposites for Photovoltaics: Interaction of the Local Structure in the Presence of Nanoparticles and the Bulk Structure

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First, how did I become a Physicist

- **A group of people that backed me up:**
  - **My maternal grandmother**
  - **My parents (who were chemists)**
  - **My high school physics teacher**

- **This helped me to know I could do whatever I wanted**

=> BS and MS at the Universidad de Puerto Rico, Recinto de Río Piedras

=> PhD at MIT

=> BMus in Music Performance at the Conservatorio de Música de Puerto Rico, then in Hato Rey, PR.

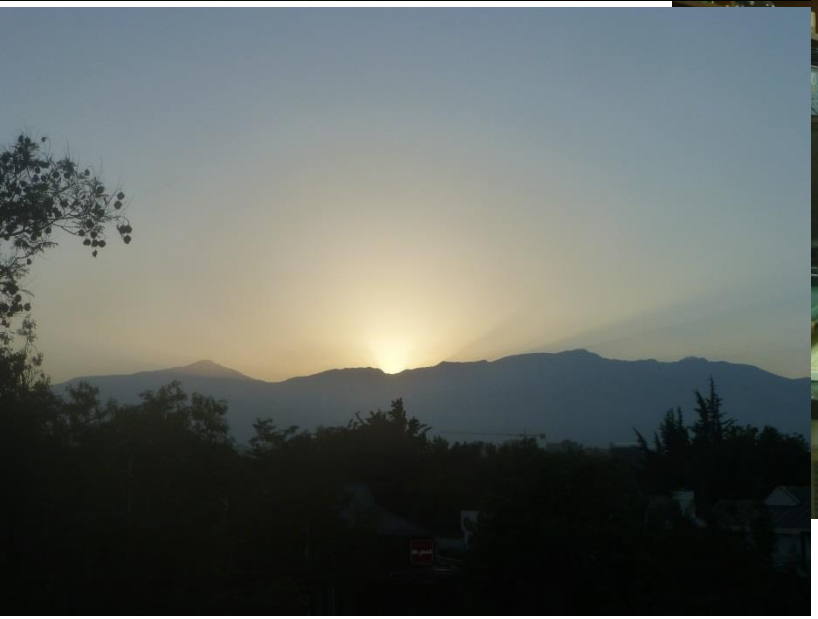
- **And it helped to remind me I could continue in Physics when I crashed…**

With the additional support of my theses advisors, don (Dr.) Fernando Díaz-Colón and Dr. Robert J. Birgeneau*

- Dr. Birgeneau advised me when I got my PhD, to "run as far away from what he did as I possibly could…"
- However, I was introduced to liquid crystals described by DeGennes (Nobel laureate) as "beautiful things"
- So I decided to go the more applied route, since my advisor followed a more basic one.
- Several times I tried to do other things, but returned to the liquid crystals, which I will be talking about in two slides.

What I like about being a physicist

- **The interdisciplinary nature of my work**
- **Meeting with people from all over the world and getting to discuss not only our work but what we like to do…**
- **Travel (this I like even outside Physics)**
- **Show my results as part of a class**



What do I do to relax…

- **Music - not always and not as often as I would like, but I try to plan to make it happen**
- **Reading – things other than physics**
- **Sewing**
- **I enjoy traveling**
- **But back to my presentation…**

Outline

1. What is a nanocomposite?

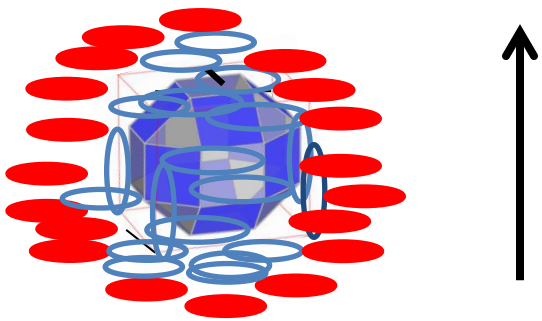
2. Why LC's?

3. Why do we subdivide the structure into two?

4. Some results – the model

5. Conclusions

What is a nanocomposite

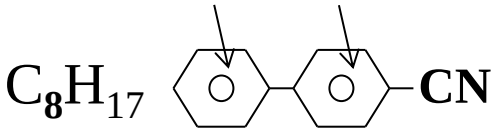


A nanocomposite is a mixture of two materials with different characteristics, that has at least one material of nanometer size. The purpose of the nanocomposite is to take advantage of the characteristics of the components.

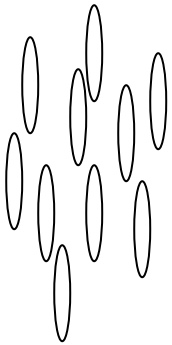
These two materials are not necessarily tied chemically to each other.

How do charges move from one material to the other?

Delocalized electrons

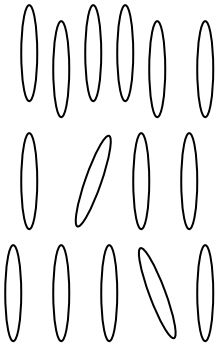


8CB, mixed with different nanoparticles

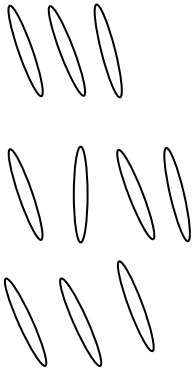


N

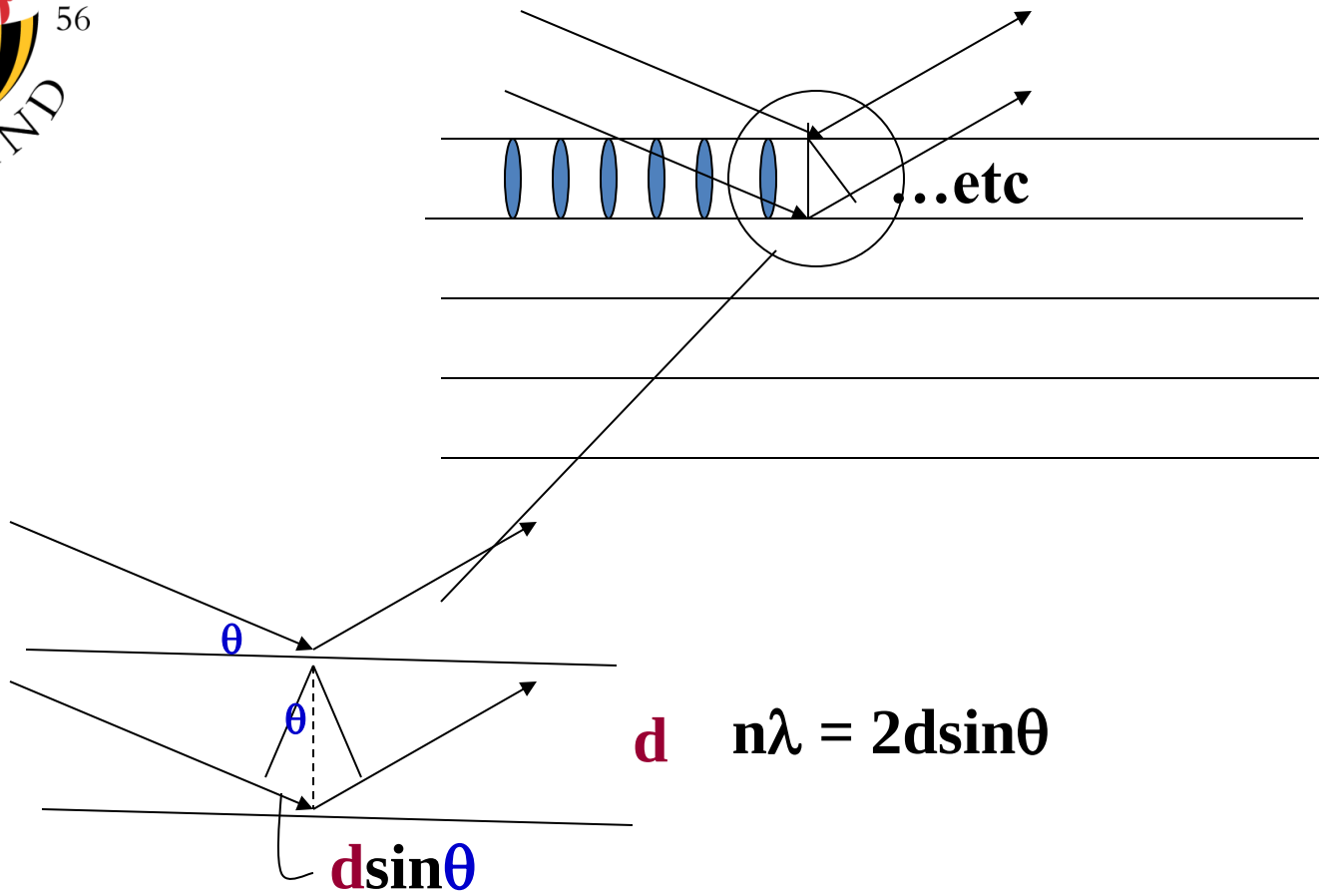
This phase has a bookshelf arrangement ➔ This gives an X-ray signal



Sm-A



Sm-C



$$n\lambda = 2d\sin\theta$$

d is in the order of 2 – 5 nm

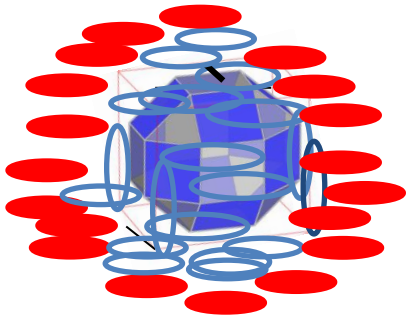
Photovoltaics

Liquid crystals are applied in photovoltaics because…

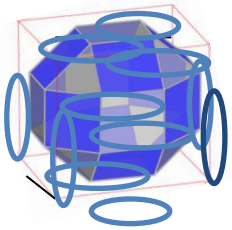
- **They self-align**
- **They have high electron mobility for organics (~10^{-5}(m^2/(Vs)))**
- **They have a large amount of delocalized electrons.**

What happens when LC are combined with nanoparticles

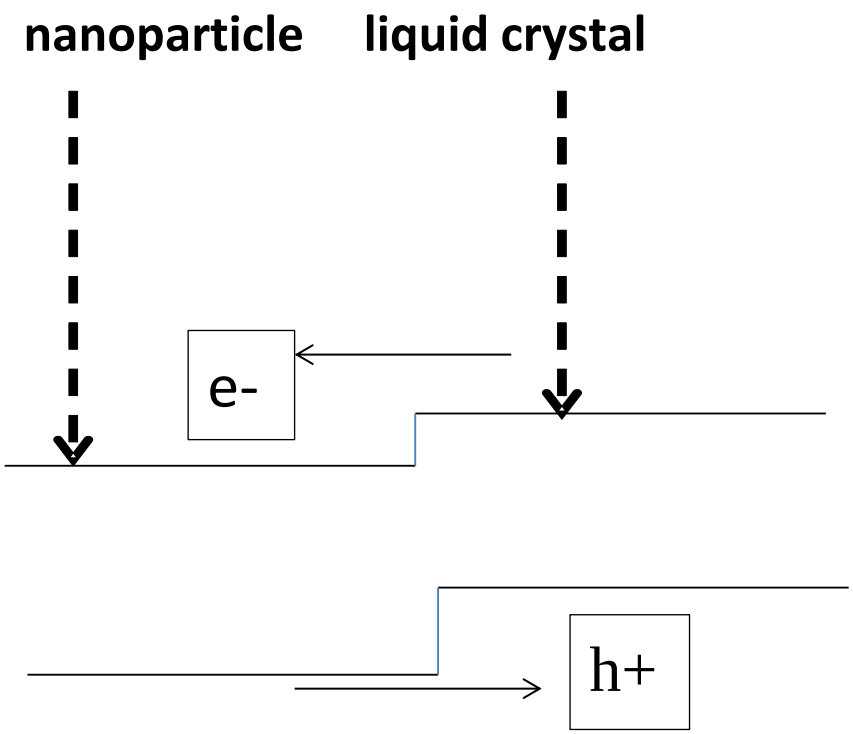
- …We use their self-alignment and the abundance of charges…



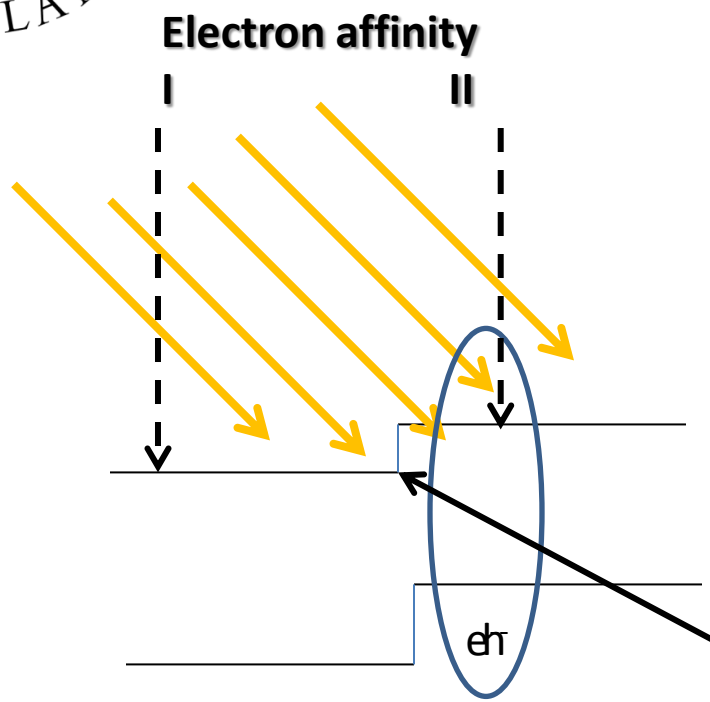
- To do this, how the liquid crystal arranges around the nanoparticle is important. Why?



There is a difference in electron affinity (ionization energy) between the liquid crystal and the nanoparticle.



This is similar to a diode



When exposed to light, they create an *exciton:*

An excited state consisting of an electron and hole bound by coulomb interactions.

What happens at this junction that allows charges to pass?

Very simplified version of model of Peumans et al,
J. Appl. Phys., Vol. 93, No. 7, 1 April 2003

To create a current:

- The exciton must be unbound

-> The distance between the e- and hole must be >= 10 nm

-> The unbinding has to happen near the <u>boundary of the two materials.</u>

Apart

Nanoparticles have a higher surface to volume ratio compared to larger particles which makes them ideal for this study…

How is this achieved

- Chemical potential yields a net current flow, with little recombination (B. A. Gregg and M. C. Hanna, J. Appl. Phys., Vol. 93, No. 6, 15 March 2003)
  - The difference between the electron affinities helps in this.

- High mobility

- Crystallinity aids in charge transport – The structure provides a path almost free of scattering centers

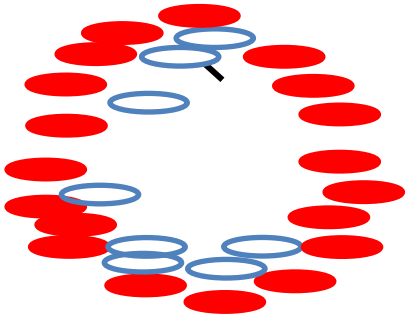
Model System

LC: 8CB

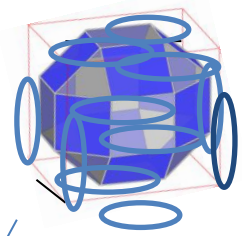
Nanoparticles:
$Fe_{48}Co_{52}$, 2 nm – several μm, with a very narrow size distribution
Or ZnO or TiO_2 ~ 3 – 6 nm
Here, we concentrate in the sizes closest to the LC.

Functionalization: PEG (polyethelyne glycol), MHDA (mercapto-hexa-decanoic acid), oleic acid, none

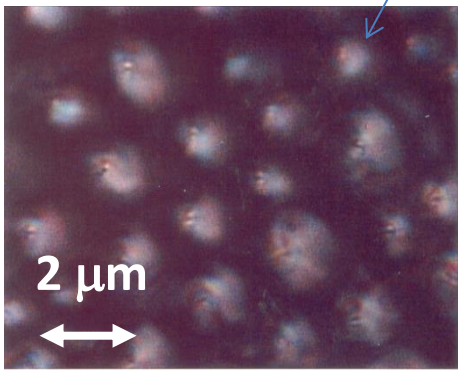
Investigate the order by using optical microscopy



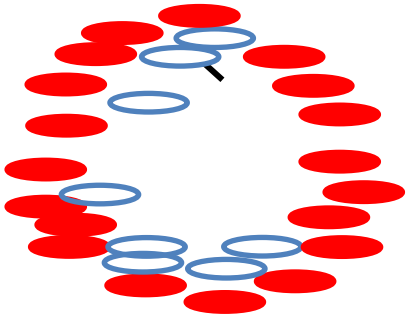
order



disorder



And X-rays



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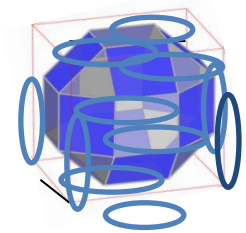

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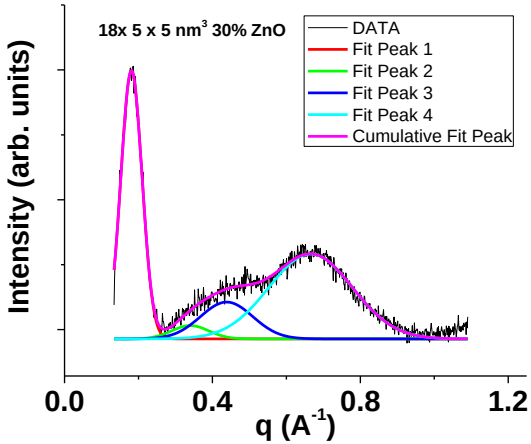
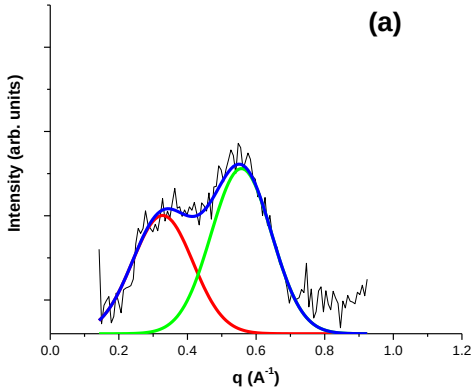
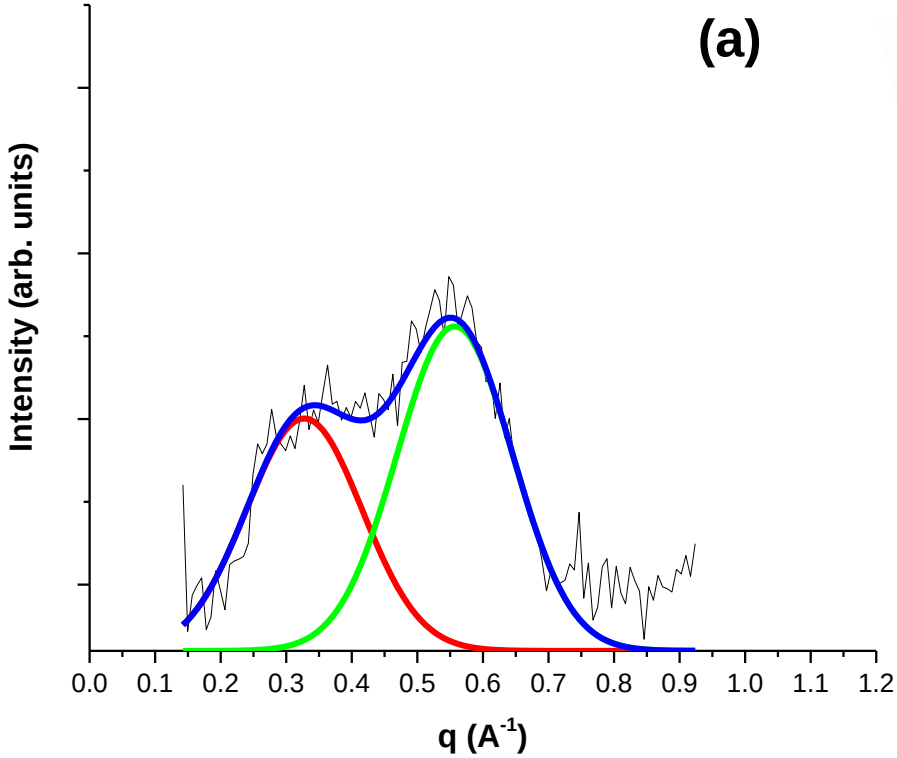
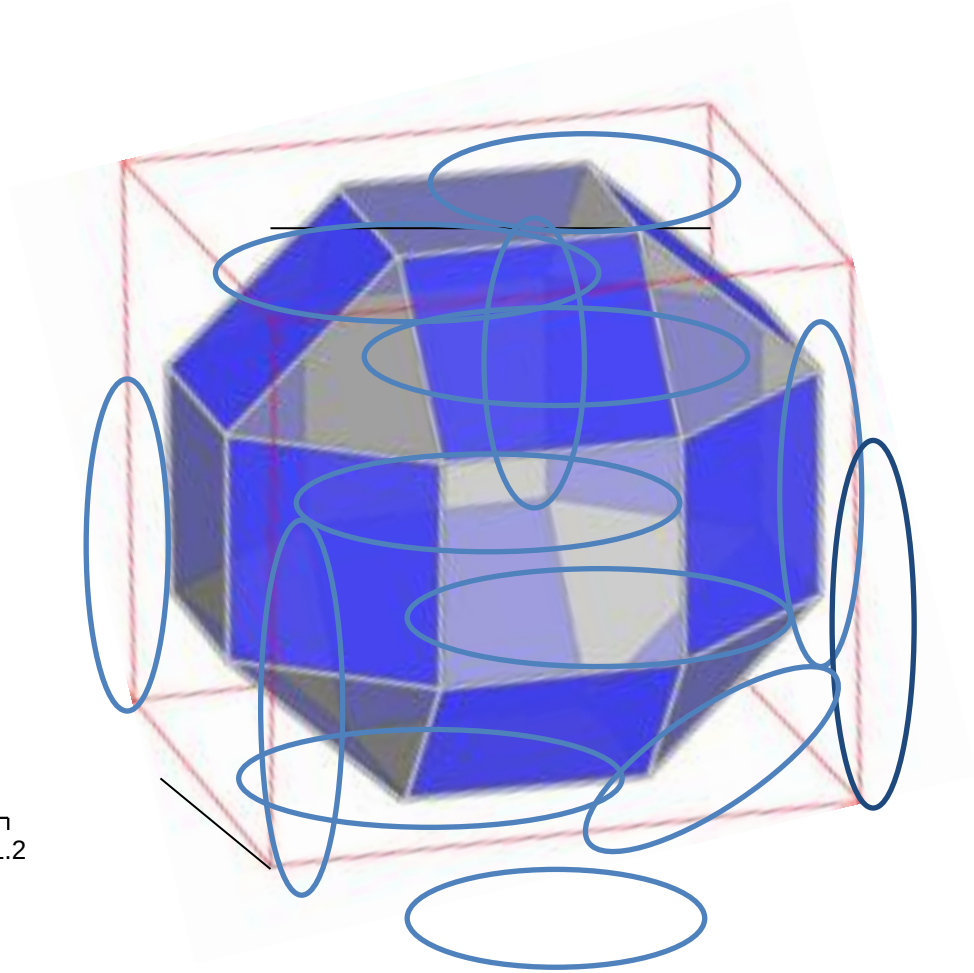




Why is it "quantized"





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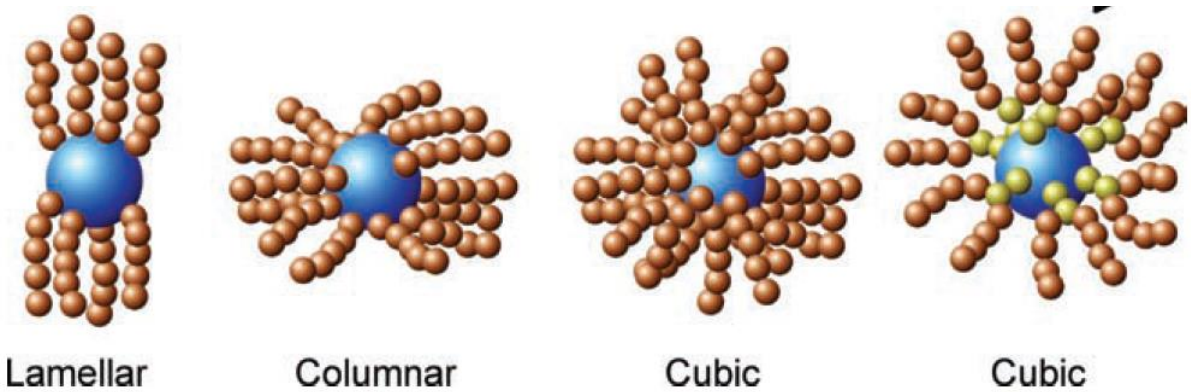
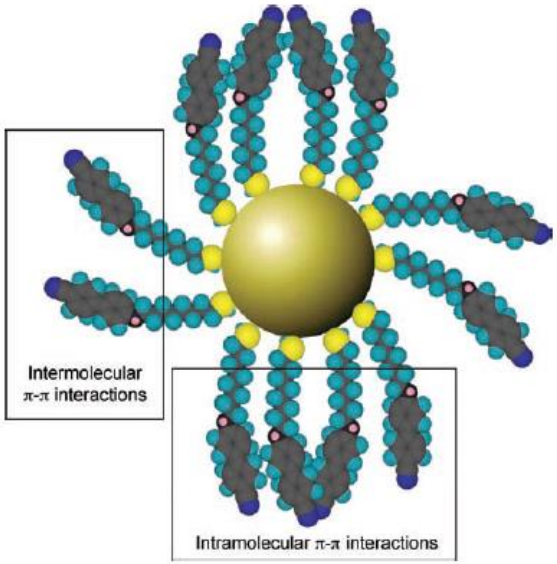
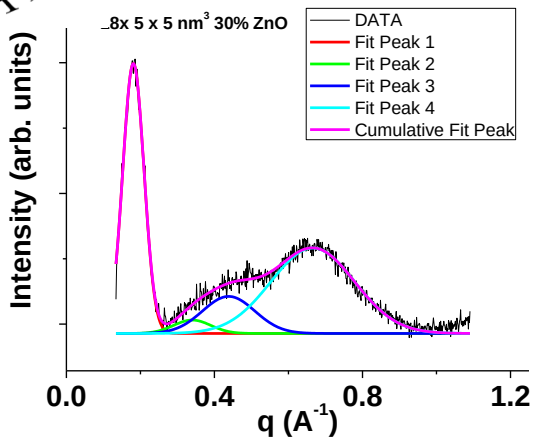
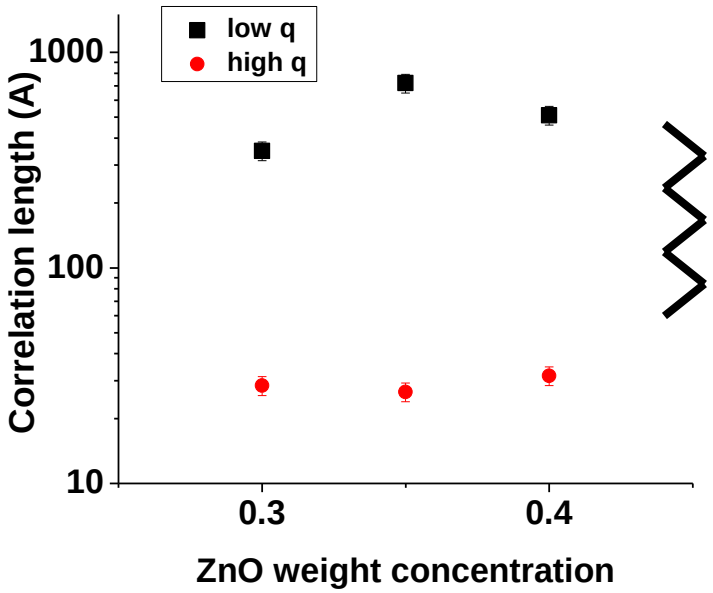


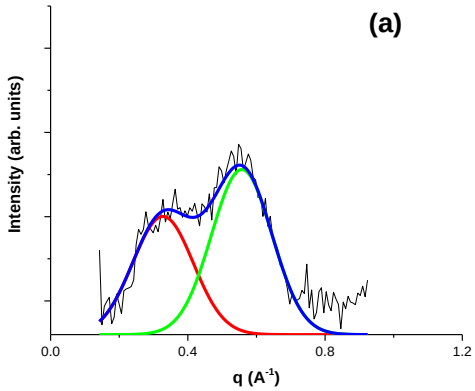
Figure 2. Effect of adsorbate density on the topology of nanoparticles and the potential mesophases that they might form.



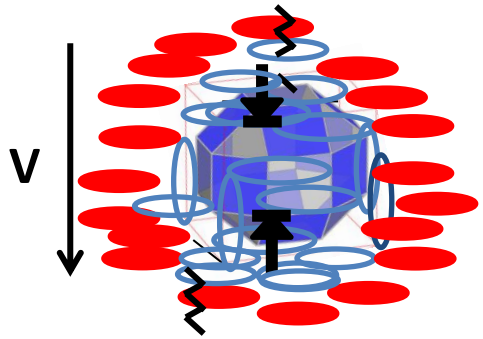
Adv. Funct. Mater. **2011**, *21*, 1260–1278







1.L. J Martínez-Miranda, et al ,APPLIED PHYSICS LETTERS **97, 223301 (2010 ; 2.** Branch, J., Thompson, R., Taylor, J.W, Salamanca-Riba, L., Martínez-Miranda, L. J., J. Appl. Phys, 115, 164313 (2014). ; 3. J. W. Taylor, Ph. D. Thesis, 2013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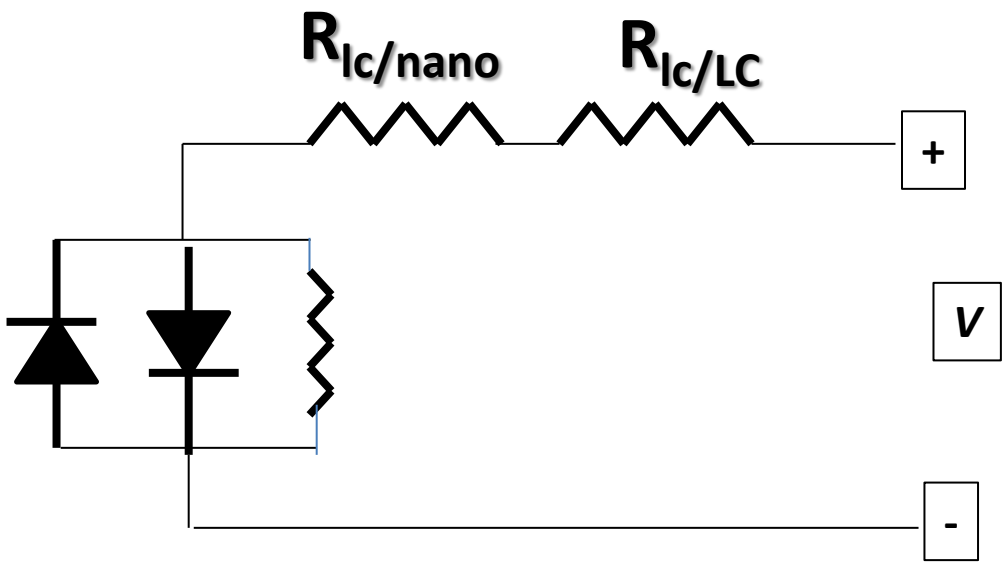
$R_{Ic/nano}$
$R_{Ic/LC}$
+
V
-

Conclusion

- Liquid crystals offer a self-aligned background that in turn aligns the nanoparticles and gives an "ordered" structure to the nanocomposites.
- The well aligned bulk associates with a not-so-well aligned liquid crystal close to the nanoparticles.
- The junction of the ordered and not-so-ordered part of the liquid crystal controls how well the charges flow into or out of the nanoparticle – Work in progress.