Experimental Report

Proposal: **9-12-319** **Council:** 4/2012

Title: Guanosine-functionalized ZnO nanoparticles for phtovoltaic applications

This proposal is a new proposal

Researh Area: Chemistry

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Samples:
poly-(p-phenylene sulfide) polymer matrix
ZnO nanoparticles + poly-(p-phenylene sulfide) polymer matrix
poly-(p-phenylene sulfide) polymer matrix
ZnO nanoparticles + poly-(p-phenylene sulfide) polymer matrix
ZnO nanoparticles + guanosine + polyadenine
ZnO nanoparticles
ZnO nanoparticles + guanosine + polyadenine + poly-(p-phenylene sulfide) polymer matrix
ZnO nanoparticles + guanosine + polyadenine + poly-(p-phenylene sulfide) polymer matrix

Instrument	Req. Days	All. Days	From	To
D22	1	1	03/12/2012	04/12/2012

Abstract:

The present research project aims to characterize a functionalized ZnO nanoparticle dispersion in a polymer matrix as active layer for solar cells. This system could represent an improvement in renewable energy field for the higher expected efficiency level. This result can be achieved coating the ZnO nanoparticles with an electron conducting molecule such as guanosine. Eventually this potential active layer is composed by a network in which nanoparticles are bound to the polymer matrix, responsible for vacancies conduction, and at the same time are connected with each other by stacking interaction between guanosine molecules. SANS investigations can help in understanding the role played by the components in determining the properties of the polymer matrix, as well as the geometrical characteristics of it.

(9-12-319-123) Functionalized ZnO nanoparticles for photovoltaic application

The performed experiment is part of a larger research project that aims to the preparation and the characterization of functionalized zinc oxide nanoparticles (ZnO NPs) as suitable system for application in very different field. In particular, recently we are interested in designing a novel functionalization for ZnO NPs, based on the introduction on their surface of bioinspired polymer, in order to obtain photoconductive layer with potential application in novel solar cell. In fact, as it is widely reported in the literature, ZnO NPs are at the same time strong absorber species in the UV region, and good semiconductors. Thus, our goal is to combine these optical and electrical properties with the optical and aggregation properties of an organic matrix obtained through the functionalization protocol. Within the final systems, the conversion efficiency of the functionalized ZnO NPs layer should be improved by an increasing yield of the electron transport, due to the coordination bond between the biopolymer and the nanoparticles surface. During this beamtime we focused on a preliminary characterization of the synthesized nanoparticle suspension, in order to investigate the shape, size, and the stability of the ZnO NPs in different suspensions. This information is fundamental in order to perform the subsequent functionalization which leads to the formation of the layer. In particular, ZnO NPs have been synthesized according to a widely reported protocol, which consists on the preparation of a zinc acetate solution in a highly alkaline medium. Keeping the solution under vigorous stirring and at the temperature of 60°C for about 1h, it is possible to observe the formation of a white precipitate corresponding to ZnO NPs. After several washing steps, the precipitate was redispersed in chloroform. ZnONPs are reported to form transparent suspension in different slightly polar solvents. Among these we choose chloroform because it was also easily available in the deuterated form, that was needed for the SANS measurements. However chloroform reveled to be not the ideal solvent for this kind of nanoparticles. In order to achieve a stable nanoparticle suspension two different sample were prepared. In one a small amount of methanol was added, since it can be physically absorbed by the nanoparticle surface and, thus, improve their stability within the suspension. On the other hand, in the second one, an amine was added as stabilizing agent. In particular, we used oleylamine, which is able to form a coordination bond between the metallic centers present on nanoparticle surface and its amino group. A set of SANS measurements was then performed on several ZnO NPs suspensions, in which the concentration of the nanoparticles and the amount of respectively methanol and oleylamine was varied. In the

figure below, two of the neutron scattering curves collected are compared. In particular, as it is shown, ZnO nanoparticle suspension in deuterated chloroform is unstable, in fact nanoparticle precipitation was observed. On the other hand, using the mixture of deuterated chloroform and deuterated methanol (90:10 w/w), a more stable suspension was obtained.

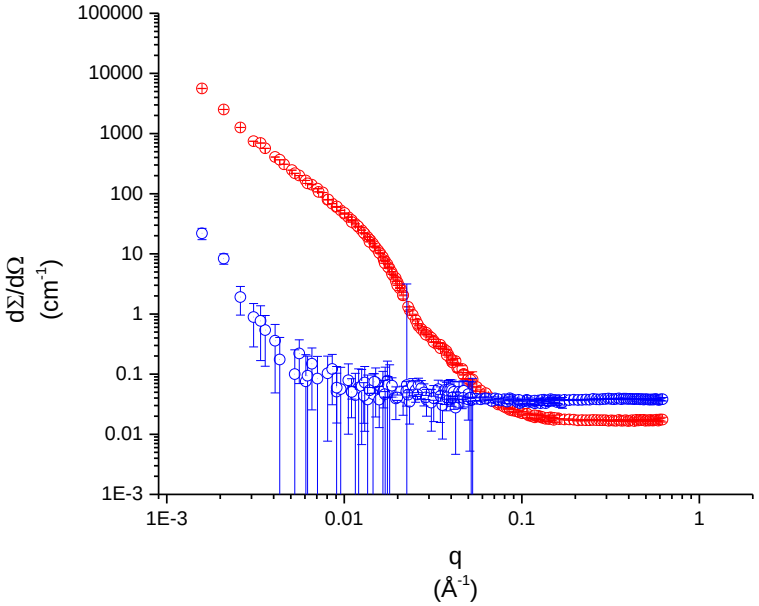

Figure: Differential scattering cross section of ZnO NPs suspensions in chloroform (blue curve) and in the mixture of chloroform and methanol , respectively 90:10 w/w, (red curve).

The analysis of this scattering profile for the stable suspensions resulted very difficult because of the rise of the differential scattering cross section at high q values, which suggest the presence in the suspension of nanoparticle clusters.

In conclusion, during this experiment, several issue concerning the nanoparticle preparation procedure rised. According to the obtained results we are now planning to modify the synthetic protocol in order to produce a more monodisperse and stable nanoparticle suspension. First successful attempt have already be done, choosing a less polar solvent still in combination with the addition of oleylamine.