2nd nanoIKER Workshop

Program & Abstracts

Tecnalia

Science & Technology Park of Bizkaia

Geldo street, building 700

10 June 2013

CIC nanoGUNE
nanoscience cooperative research center

tecnalia
Corporación Tecnológica

nanoIKER project

ETORTEK funded by the Department of Industry, Innovation, Trade, and Tourism of the Basque Government

Project leader:

Participants:

Program

08:00 Registration

08:30 Welcome

08:45 SAMOKEM. "Quantitative Magneto-Optical Characterization of Diffusive Reflected Light from Rough Steel Samples Acquired with the SAMOKEM Tool", J. Gonzalez (nanoGUNE)

09:15 POLYMERS. "PU/acrylic waterborne hybrid adhesives: Structure and properties", P. Carretero (UPV/EHU-POLYMAT) and G. Martinez-Rugerio (CFM)

09:45 PHOTON. "Scattering and Near-field of infrared nanoantennas", P. Alonso (nanoGUNE)

10:15 BASKRETE. "Shear deformations in the C-S-H gel: understanding the molecular mechanism of creep", H. Manzano (UPV/EHU)

10:45 GRAPHENE. "Exfoliation of graphene oxide using ionic liquids: experimental and molecular modelling approach", B. Coto (IK4-TEKNIKER)

11:15 Coffee Break – poster session

11:30 EnergiGUNE. Teófilo Rojo (Invited talk)

12:15 MicroGUNE. Enrique Castaño (Invited talk)

13:00 Lunch – poster session

15:00 SAMOKEM. "Focused electron beam induced deposition and magneto-optical magnetometry of cobalt nano-structures", O. Idigoras (nanoGUNE)

15:30 POLYMERS. "Nanostructuring of thermosetting matrices with different block copolymers", G. Kortaberria (UPV/EHU-GMT)

16:00 PHOTON. "Influence of Quantum effects on Plasmonic systems", R. Esteban (CFM-DIPC)

16:30 Coffee break – poster session

16:45 BASKRETE. "Theoretical 29Si NMR in hydrated Portland cement", P. Rejmak (DIPC)

17:15 GRAPHENE. "Water-borne graphene/polymer composites: colloidal stability issues", A. Arzac (UPV/EHU-POLYMAT)

Posters

P1 "Graphene-triazolium π-π interactions: a computational and experimental study", J. M. Aizpurua (UPV/EHU)

P2 "PI-b-PMMA diblock copolymers: nanostructure development in thin films and nanostructuring of thermosetting epoxy systems", I. Barandiaran (UPV/EHU-GMT)

P3 "Hybrid miniemulsion photopolymerization in continuous tubular reactor", V. Danilovska (UPV/EHU-POLYMAT)

P4 "Improvement in the design and prototype fabrication of a Stand-Alone Magneto-Optical Kerr Effect Magnetometer", A. Lasaosa (CEIT-IK4)

P5 "Water-borne graphene based electrically conductive adhesives", G. P. Leal (UPV/EHU-POLYMAT)

P6 "Hybrid nanophotonic structures: synergy between inorganic and organic materials", D. Melnikau (CFM)

P7 "Liquids on the nanoscale: Electrospinning from free jets, and confinement in tubes", A. Rebollo (nanoGUNE)

P8 "Aqueous phase exfoliation of graphite by cellulose nanocrystals", V. Ruiz (IK4-CIDETEC)

P9 "Coupling light from a photonic crystal waveguide to metallic transmission lines in the mid-IR", P. Sarriugarte (nanoGUNE)

P10 "Fabrication of Magnetic Battlements", N. Soriano (UPV/EHU)

P11 "Stable colloidal dispersions as a valuable tool for self-assembling of graphene platelets in polymer matrix", R. Tomovska (UPV/EHU-POLYMAT)

P12 "Correlative infrared-electron nanoscopy reveals the local structure-conductivity relationship in zinc oxide nanowires" (IK4-CIDETEC)

Talks

SAMOKEM

Quantitative Magneto-Optical Characterization of Diffusive Reflected Light from Rough Steel Samples Acquired with the SAMOKEM Tool

J.B. González-Díaz[1], J.A. Arregi[1], A. Martínez-de-Guerenu[2], F. Arizti[2] and A. Berger[1]

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Magneto-Optical Kerr Effect (MOKE) magnetometry, spectroscopy and ellipsometry have been employed to characterize and study magnetic systems with different types of surfaces including rough ones [1-6], where it has been shown that there is an important relation in between surface roughness on one hand and domain size and magnetization reversal on the other [1-2,4]. The study of this kind of surfaces is of great importance to achieve a better understanding of the macroscopic magnetic response that arises from complex surfaces and its application to all types of devices. However, up to now, all magnetic-optical studies have focused on surfaces where two fundamental characterization parameters, namely average roughness R_a and mean peak spacing RS_m, are small in comparison to the wavelength of light [1-6]. To our knowledge, no study has analyzed the magneto-optical response in other roughness regimes, i.e., magnetic surfaces with roughness parameters of the order (or much larger) than the wavelength of light, that makes the reflected light show a diffusely broadened spot. The only exception, being a very special case of roughness, is the study of the magneto-optical (MO) response of diffracted beams for samples, in which the surface has periodic variations [7,8]. This lack of studies may be attributed to the fact that diffuse light is not only very difficult to measure but also challenging to interpret for generalized geometries, since the measurements usually depend on the spot size collected at the photo-detector as well as on the different optical and magneto-optical responses that occur at different scattering angles [7,8].

An analysis of samples with significant roughness would be useful from an applied and industrial point of view, since it may allow a low-cost non-invasive surface magnetic characterization of industrial samples. This is precisely the purpose of the SAMOKEM project, which aims at achieving an understanding the MO response from complex magnetic surfaces, besides developing a portable, compact and efficient tool for MO measurements. Specifically, we measure here the magneto-optical response of polished industrial samples of varying average roughness R_a, which is of the order of the light wavelength and has a mean peak spacing RS_m that is much larger than the observation wavelength (see figure 1). For this purpose, we performed quantitative MOKE measurements for diffusely scattered light with high signal-to-noise ratio using the table-top experiment developed for the SAMOKEM prototype. Our study demonstrates that for these specific samples, the magneto-optical activity is monotonously increasing as a function of the scattering angle, while preserving its field dependent shape, i.e. the hysteresis loop shape (see figure 2). We furthermore find that this behavior can be explained by considering the diffused light reflected from a rough surface to be equivalent to the reflection of light from planar surface segments with varying incidence angles. These results demonstrate the potential applicability of the SAMOKEM tool for the analysis of rough surfaces and therefore, we conclude that this kind of quantitative magneto-optical characterization has the potential to find wide-spread applications in industry.

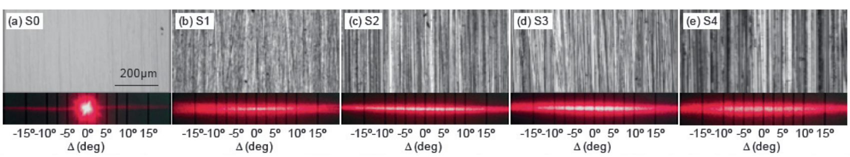

Figure 1. Light microscopy images of the different samples employed in this study. For the sake of roughness comparison, all sample stripes are aligned vertically. The scale shown in (a) applies to all pictures. Below the images, we show the scattered laser spots corresponding to each of the samples. Δ accounts for the difference in between incidence and scattering angles (Δ = 0 for specular reflection).

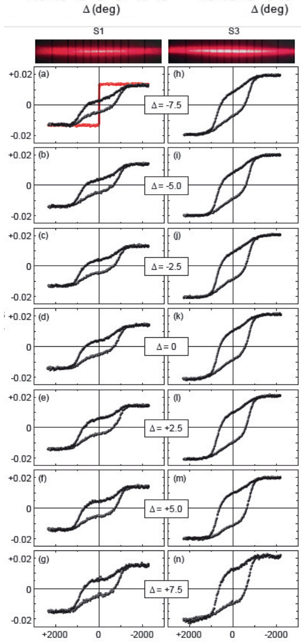

Figure 2. Experimentally determined Kerr rotation hysteresis loops for different scattering angles: (a-g) sample S1 with small roughness; (h-n) sample S3 with larger roughness. For comparison, figure (a) also displays the normalized bulk magnetization response of sample S1 (which is equivalent for all samples in our study) as a function of the applied magnetic field.

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POLYMERS

PU/Acrylic waterbone hybrid adhesives: structure and properties

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Waterborne PU/acrylic hybrid adhesives have been synthesized by miniemulsion polymerization. Two different initiation strategies have been used; thermal initiation at 70ºC and photoinitiation at 25ºC. The nanostructure obtained with both types of initiations as well as varying the process variables in the case of photopolymerization has been studied, as well as its effect on the final adhesive properties of the hybrid systems.

PHOTON

Scattering and Near-field of infrared Nanoantennas

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Light scattering at nanoscale objects - such as particles and molecules - can be dramatically enhanced in the "hot spots" of plasmonic antennas, where the incident light is highly concentrated. Although this effect is widely applied in surface- and field-enhanced optical sensing, spectroscopy and microscopy, the underlying electromagnetic mechanism of the signal enhancement has not yet been traced experimentally. To this regard, in this contribution we will present a new approach to resolve the role of the antenna in the scattering process by studying the elastically scattered light from an individual object located in the well-defined hot spot of single antennas. Understanding scattering processes in optical and IR nanoantennas is crucial to develop field-enhanced spectroscopy, effective biosensors and control of coherence in quantum emitters, among other applications..

BASKRETE

Theoretical ^{29}Si NMR in Hydrated Portland Cement

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Hydrated Portland cement consists of 50–70 % in mass of calcium–silicate–hydrate (C–S–H) gel, an amorphous solid responsible for most of the cement mechanical properties [1]. Although C–S–H gel is the most widely manufactured material in the world, its exact nanostructure is not fully explained yet. The present atomistic models of C-S-H gel are based on two layered inosilicate minerals, either jennite or tobermorite [2]. ^{29}Si MAS NMR is one of the most commonly used experimental technique for the characterization of C–S–H gel [3]. However, NMR results are not able to unambiguously elucidate the structure of this complex material.

We here present the first, up to the best of our knowledge, theoretical simulation of ^{29}Si MAS NMR spectra for the structural models of C–S–H gel [4]. Magnetic shielding tensor was calculated at the density functional theory level employing Gauge Including Projector Augmented Waves

method [5]. The chemical shifts was obtained using selected silicates as the references. In order to simulate NMR spectra of amorphous C–S–H gel we sampled fifteen different periodic models, derived from the experimental structures of jennite and tobermorite. We found the best agreement between calculated and experimental MAS NMR spectra of C–S–H gel for tobermorite based models with high Ca loading. We also investigated ^{29}Si chemical shift anisotropies and showed that this quantity can discriminate various Si sites in C–S–H gel in much clearer way than isotropic chemical shift only [6].

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GRAPHENE

Exfoliation of graphene oxide using ionic liquids: experimental and molecular modelling approach

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Graphene, a one-atom-thick planar sheet of sp^2 hybridized carbon, has received much attention due to its outstanding properties such as large specific surface area, high electrical and thermal conductivity, excellent chemical stability and mechanical stiffness. Graphite, which is cheap and readily available, consists of stacked graphene sheets. Therefore, one of the most convenient methods for the mass production of graphene sheets is the exfoliation of graphite in the liquid phase. Recently, many attempts to produce graphene sheets in large quantities via chemical reduction of exfoliated graphite oxide (GO) have been reported. During the oxidation process of graphite, the unique electronic properties of graphene dramatically degrade. The electrical conductivity of the graphene oxide sheets can be partially restored by the reduction step; however, this results in their irreversible agglomeration. Therefore, different strategies to disperse graphene sheets before or during reduction step have been used, including stabilization by various polymeric dispersants or surfactants and covalent/non-covalent functionalization [1].

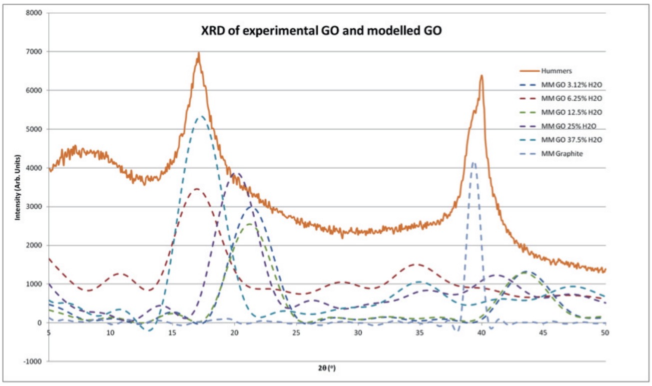

Figure 1. XRD Experimental and simulated patterns of graphite oxide.

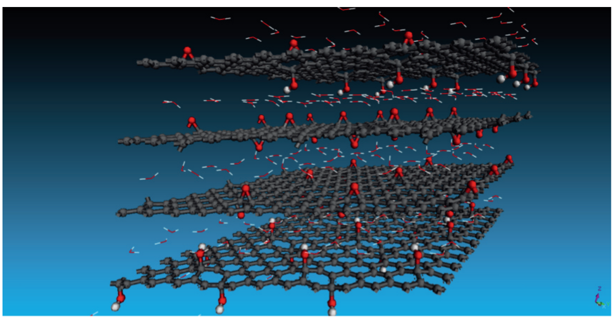

Figure 2. Molecular model of graphite oxide with adsorbed water.

In this context, ionic liquid (ILs) can be used for functionalization of graphene. They can adsorb on the graphene surface through the noncovalent interactions of anion and/or cation with graphene. ILs present several advantages such as enhanced ionic conductivity, thermal stability and excellent mechanical properties. The graphene modified with ILs are endowed with improved conductivity, excellent hydrophilicity and positive charged [2]. The repulsion between the resultant cation-charged GO sheets, the charge transfer between the ions and graphene and the high solubility of the grafted IL contribute to the exfoliation of graphite into graphene sheets and to prepare long-term stable graphene dispersions using ILs [3].

In this work, several ILs with different chemical structures have been synthesized and employed for the modification of graphite and graphite oxide in order to show the possible exfoliation of graphene layers in both materials. The graphite oxide employed for the study has been prepared by the Hummers method. The average interlayer spacing between the exfoliated graphene layers in graphite and graphite oxide has been measured by X-ray diffraction (XRD) (figure 1). Molecular dynamics simulations were also used to study the influence of ILs in the interlayer spacing (figure 2).

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SAMOKEM

Focused electron beam induced deposition and magneto-optical magnetometry of cobalt nano-structures

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The ability of fabricating and characterizing nanostructures with high precision is of crucial importance for a wide range of technological applications, such as for instance, in semiconductor industry. Even though structuring of nanoscale systems may be achieved by different lithography techniques [1], focused electron beam induced deposition (FEBID) has recently attracted a very substantial amount of interest [2,3]. FEBID is based on the electron-induced dissociation of a molecular precursor gas into volatile and non-volatile components, which then deposit onto surfaces [3,4]. One of the most attractive features of this technique is the rapid prototyping, because it is a one-step technique. Moreover, FEBID allows for the fabrication of 3-dimensional complex nanostructures in a wide range of materials. In this work, we have fabricated several Co nanostructures by means of FEBID, including wires where lateral dimensions were shrunk down to 30 nm, as well as 3 dimensional nano-pillars. Their magnetic properties have been measured by means of a magneto-optical Kerr effect (MOKE) microscopy [5], which is a powerful technique to image magnetic domains, as well as characterize individual properties of magnetic nanostructures. Thus, this work is tightly connected to the SAMOKEM project of nanoIKER.

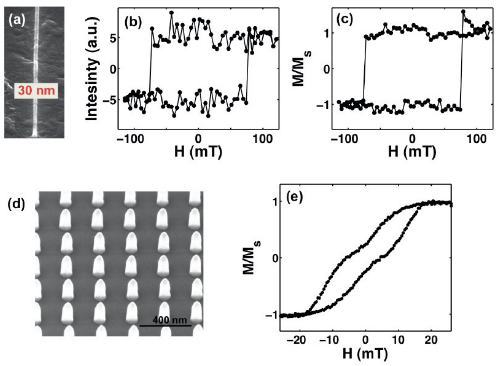

Figure 1: (a) and (d) show scanning electron microscope images respectively of a 30 nm wide Co wire and an array of nanopillars of size 80 x 210 nm, both of which are fabricated by electron beam induced deposition. (b), (c) and (e) display hysteresis loops measured in these structures by Kerr effect microscopy. While (b) and (c) show hysteresis loop measured for the 30 nm wide Co wire ((b) is a single shot measurement and (c) an average of 9 loop cycles), (e) shows the hysteresis loop measured for the Co nanopillar array in (d).

FEBID of Co structures has been done by using a commercial Helios NanoLab™ DualBeam™ system (FEI, Netherlands). Figure 1 (a) shows a scanning electron microscopy image of a 30 nm wire, while figure 1 (e) displays an array of pillars that are 80 nm wide and 210 nm high. In order to get the right composition, lateral resolution and desired shape of the structures one needs to find the optimal deposition parameter conditions. Both structures were made at constant values of background pressure (6×10^{-5} Pa), step size (5 nm) and sample to gas injection system distance (50 μm). While the 30 nm wide wire was produced using a high electron beam energy of 30 kV, an electron beam current of 2.7 nA and 6×10^{-5} Pa precursor gas pressure, the nanopillars were obtained by using an electron beam energy of 2 kV in conjunction with an electron beam current of 86 pA and 8×10^{-4} Pa precursor gas pressure.

The magnetic analysis was carried out with an optical wide-field polarization microscope optimized for Kerr microscopy (Evico Magnetics GmbH, Germany). The microscope is equipped with a high sensitivity CCD camera that is capable of taking magnetic-contrast images down to 25x20 μm² sample surface areas, divided into 1024x768 pixels. The key feature of our approach is that we can measure the field dependent local magnetization, either in-plane or out-of-plane, by selecting an arbitrary (shape, size, and position in the field of view) region of interest (ROI) on the CCD camera pixel array, and use this array selection as a conventional light intensity detector. In this way, we can maximize the magneto-optical signal, resulting in an optimized signal-to-noise (S/N) ratio. The advantage of our approach is evident from the measurement reported in Fig. 1(b), where we demonstrate that we are able to record a single shot hysteresis loop with an average S/N of 4.1 per data point for a 20 nm high Co wire that is only 30 nm wide (Fig. 1 (a)). Renormalizing this result to the commonly used detection criterion (S/N = 2), we conclude that our measurements are sensible to a magnetic moment of only 2×10^{-15} Am². By comparing our results to other magnetometry techniques such as the latest generation SQUIDs with their sensitivity in the 10^{-12} - 10^{-13} Am² range, it becomes obvious that MOKE microscopy based magnetometry allows for true nanoscale magnetic characterizations. Figure 1 (c) shows an average over 9 single shot measurements for the 30 nm wide wire. Here, we find that the S/N has increased by a factor of almost 3. This confirms that we could measure even smaller structures with less than 10 nm width.

For the 30 nm wide wire, one observes a rectangular hysteresis loop with a coercive field of 75 mT (Fig. 1 (c)), i.e. the expected behaviour given that the external field is applied along the wire length, which is the easy axis of magnetization due to shape anisotropy. In the case of hysteresis loops measured in a periodically ordered 20 x 20 nanopillar array (Fig. 1 (e)), a center-pinched structure is found with reduced magnetization in the remanent state and a plateau-like feature at low applied fields, i.e. a behavior that arise due to the magnetostatic coupling between adjacent pillars if exchange coupling is low or absent.

Our results demonstrate that the combination of FEBID and MOKE microscopy makes it possible to explore magnetization reversal properties of individual and collective nanostructures andthus opens up a broadly applicable avenue to perform systematic research on nano-scale magnets.

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POLYMERS

Nanostructuring of thermosetting matrices with block copolymers

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Nanostructuring of epoxy thermosetting matrices with block copolymers has been carried out by using different types and amounts of block copolymers such as poly(styrene-b-butadiene-styrene) (SBS), poly(styrene-b-ethylene oxide) (PSEO) or poly(isoprene-b-methylmethacrylate) (PI-b-PMMA). Different morphologies have been obtained depending on the copolymer amount and curing conditions. The effect of block copolymers on the cure reaction kinetics has been also analyzed. Obtained nanostructures have been used for the selective placement of nanoparticles in the generated nanodomains.

PHOTON

Influence of Quantum effects on Plasmonic systems

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Metallic particles of nanometer dimensions support plasmonic resonances at optical and infrared frequencies, which are often exploited to obtain very strong and localized near fields. A system of particular interest is a dimer consisting of two particles separated by a very narrow gap. For most practical purposes, this system can be studied classically, describing the material by its permittivity and solving the Maxwell equations. However, for subnanometer separation distances quantum tunneling can strongly modify the optical response, changing the modal structure and suppressing the intensity of the local fields at the gap. Here, we discuss the behavior of dimers on these classical and quantum regimes, and discuss a simple method developed to include the influence of quantum tunneling on calculations of large plasmonic system. We last discuss recent experimental results demonstrating the emergence of the quantum effects on plasmonic systems with very narrow gaps. Quantum effects might be crucial in a variety of applications ranging from field-enhanced spectroscopies to biosensing and microscopy technologies involving the subnanometric scale.

BASKRETE

Molecular modelling of shear deformations in ordered and disordered Calcium Silicate Hydrates

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UPV/EHU

The calcium silicate hydrate (C-S-H) gel is the phase that provides cohesive strength to cement. The mechanical properties of the C-S-H gel at the molecular level are key to the durability of infrastructures made of concrete, controlling macroscopic properties such as creep. Unfortunately, the existing experimental techniques cannot access the nanostructure and properties of this very heterogeneous phase, which implies a lack of understanding on the molecular scale mechanisms governing creep. Under this scenario, atomistic simulations constitute a valuable alternative. In this work we study the mechanical response of a C-S-H gel disordered model under large shear deformations using reactive force field simulations. First, we calculate elastic properties of the system. Then we apply deformations beyond the elastic limit, analyzing the localization of stresses and strains. Our results point to the importance of water in creep, so we complement the study simulating systems with different water contents. Finally, the energy barriers under strain are employed to link the strain and time for the material. Implications of our findings for a colloidal description of the C-S-H gel mechanics and for the macroscopic properties of cement are discussed.

GRAPHENE

Water-borne graphene/polymer composites: colloidal stability issues

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UPV/EHU-Polymat

We present synthesis of water borne polymer graphene composites for possible application as electrically conductive coatings in the next-generation material for nanoelectronic devices. Since the colloidal stability of the prepared hybrid dispersions is an issue of great significance for water borne products, it was performed a systematic study toward stable colloidal aqueous polymer/graphene hybrid latexes, capable to form composite films by water evaporation at standard atmospheric conditions. The main route that was followed is to stabilize firstly the graphene nanoplatelets (GNPs) or reduced graphene oxide (rGO) in water by means of different surfactants following liquid phase exfoliation procedure (LPE), composed of subsequent sonication and centrifugation. Starting from these stable graphene aqueous dispersions, water borne polymer hybrid dispersions were prepared by two procedures: emulsion mixing (blending) and in situ polymerization. The selected polymer system is composed from poly(methyl metacrylate/butyl acrylate) in 50/50 wt% ratio in order to obtain glass transition temperature (Tg) of the final film lower than room temperature. The semicontinuous seeded emulsion polymerization has been used to prepare the polymer nanoparticles aqueous dispersions (latexes) to be used for emulsion mixing, and to prepare hybrid latexes by in situ reactions. Very stable hybrid dispersions were prepared, which have shown to be a valuable tool toward composite films containing highly ordered rGO platelets in the polymer matrix.

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