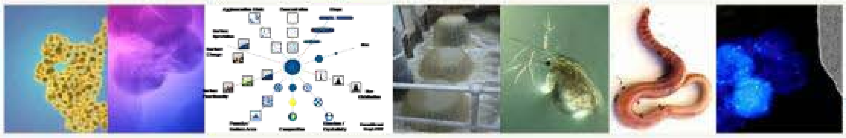


Component 1 Particle Chemistry and Fate

The work is centred on refining the production of engineered nanoparticles (ENPs).

Component 1 studies and methodological development contribute to:

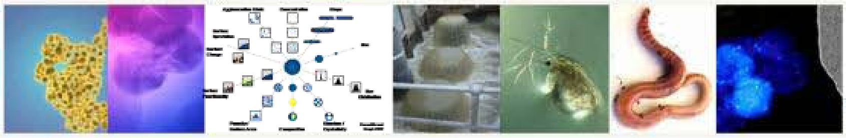
Workpackage 1	Workpackage 2
Characterisation and Tracking of ENPs during processes involved in fate and toxicity	ENP Environmental Behaviour and Fate Modelling

Visit the NanoFATE Workpackage descriptions

Many questions within WP 3, 4, 5 are related, and data from all three WPs are needed to gain understanding of the ecotoxicology and bioavailability of Zinc Oxide (ZnO) and Silver (Ag) nanoparticles.

Meet the PhD and PostDoc students conducting research for NanoFATE Component 1:

Julián Gallego	Fate of Nanoparticles: Aggregation Kinetics and Adsorption of Macromolecules
Agnieszka Opalinska	Stability of Nano-ZnO Suspension as a Function of pH; Zetasizer – a Tool for Measurement of Stability, Solubility and Aggregation of Nanopowders
Cameron Taylor	Characterisation of Engineered Nanoparticles and Their Interaction with Natural Biological and Nonbiological Surfaces
Jacek Wojnarowicz	Solvothermal Synthesis of Nanocrystalline Zinc Oxide Doped with Co and Gd



Julián Gallego

UGOT
Dept. of Chemistry

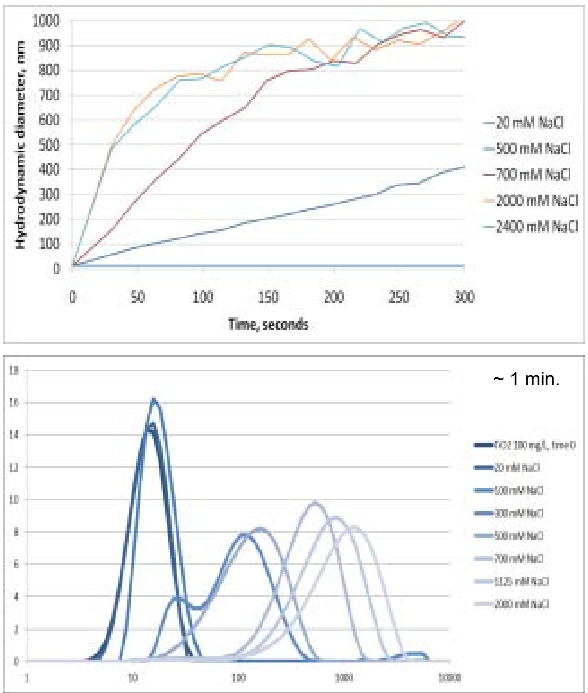
Fate of Nanoparticles: Aggregation Kinetics and Adsorption of Macromolecules

Julián Alberto Gallego-Urrea graduated from the National University of Colombia in 2000 with a BSc in chemical engineering (contributing to the design of a municipal wastewater treatment plant). He obtained an MSc in civil and environmental engineering in 2003 from the University of Los Andes (Bogotá). His dissertation was focused on the use of water quality models for risk analysis regarding introduction of toxic substances into drinking water network systems. His DPhil with Dr Martin Hassellöv at the University of Gothenburg relates to environmental chemistry and ecotoxicology of ENPs.

UNIVERSITY OF GOTHENBURG

NanoFATE is focused in a novel field of study dealing with environmental risk assessment of manufactured nanoparticles, with emphasis on Environmental Chemistry and Ecotoxicology. My work for the project deals with NP characterisation and evaluation of interactions with natural water; routes of exposure for ecotoxicological tests; and fate of nanoparticles in the environment. The slides below give a glimpse of my approaches and the data that are already emerging.

NP aggregation studies
Determining attachment efficiency, α:

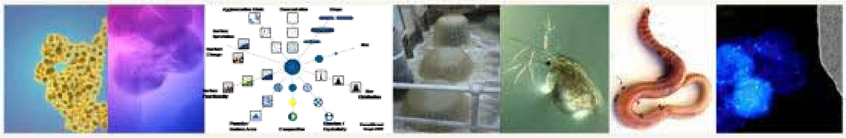


Measuring the increment in size using Dynamic Light Scattering (DLS) provides qualitative information on the stability of NP dispersions. This allows us to calculate attachment efficiencies, α, as an indicator of the degree of destabilization.

$$\alpha = \frac{\left(\frac{d(R_h(t))}{dt}\right)_{t\to 0}}{\left(\frac{d(R_h(t))}{dt}\right)_{t\to 0,\, fav}}$$

α: fraction of collisions that lead to attachment

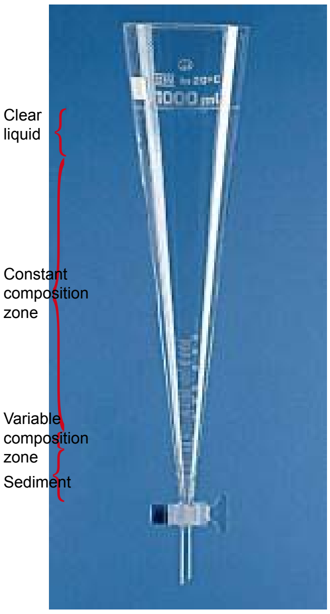
Julián Gallego



Julián Gallego

UGOT

Sedimentation vessels (Imhoff)



Contribution to Nanofate: Sedimentation rates and influence of velocity gradients and different water chemistry.

- Sedimentation rates and basic settling characteristics can be determined for concentrated (particle-particle interactions not neglected) fine particles.
- Sampling in intermediate points (and sediment) allows to examine layer characteristics at a given time.
- UGOT has built 4X6 sets of settling vessels and has a Master's student now starting to work with this.

Dissolution experiments

- Both Zinc oxide and silver nanoparticles are prone to dissolution
- I'm now developing a simple method for measuring dissolution rates based on centrifugal ultrafiltration and elemental analysis (ICP-MS)

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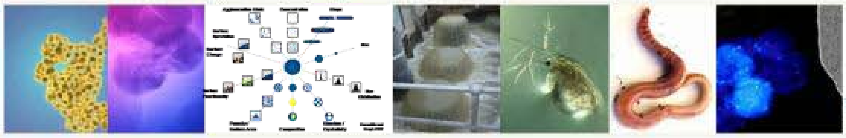

Agnieszka Opalinska

Stability of Nano-ZnO Suspension as a Function of pH; Zetasizer – a Tool for Measurement of Stability, Solubility and Aggregation of Nanopowders

Inst. of High Pressure Physics, Polish Academy of Science

Agnieszka Opalinska graduated from Warsaw University of Technology in the field of Chemical Technology, with a major in Ceramic Technology. Her Master's thesis was entitled 'Synthesis of nanocrystalline TiO2 for self-cleaning coatings'. Currently she is working with Prof. Witold Łojkowski at Institute of High Pressure Physics of the Polish Academy of Science on her doctoral thesis, which is dedicated to synthesis and characterization of nanoparticles.

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The main subject of my work in NanoFATE is the synthesis and characterization of doped nano-zinc oxide, with special focus on the study of the stability of nano-ZnO suspension. I take care of synthesizing and characterizing our particles (nano-ZnO doped with Co and Gd), and I'll use the MALVERN Zetasizer Nano-ZS, a system with automatic titration, to study suspensions stability.

My work will answer the following questions:

- *What is the agglomerate size and stability of suspension of nano-ZnO doped with Co and Gd in different types of water?*
- *What are similarities and differences between our nano-ZnO and that produced by commercial concerns (Nanosun, Basf...)?*

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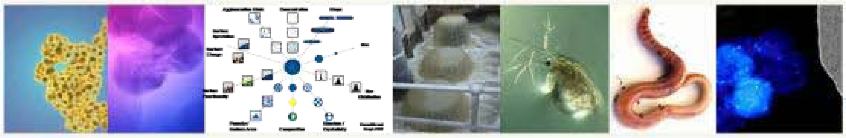


Cameron Taylor

University of Oxford-Materials

Characterisation of Engineered Nanoparticles and Their Interaction with Natural Biological and Nonbiological Surfaces

Cameron Taylor graduated from Edinburgh University with a BSc in Environmental Geoscience. His dissertation focused on the toxicity of Ag and ZnO nanoparticles to two different bacterial strains. He recently completed a Masters in Environmental Sustainability, also at Edinburgh. He is working with Dr Alison Crossley at University of Oxford Materials Department on his DPhil which relates to nanoparticle characterisation.

OxfordMaterials

UNIVERSITY OF OXFORD

My project will focus on characterisation of the particles used in NanoFATE (Ag, ZnO and CeO2) using a selection of different experimental techniques:

• Dispersions are studied using DLS, NTA, differential centrifugation and TEM – the particle size distribution, shape and charge effects will affect the state of the particles and the stability in a nanoparticle dispersion

• The interactions of the particles with laboratory glassware are studied using Raman and UV-Vis spectroscopy.

I am using, or training to use, a number of key techniques:

Dynamic Light Scattering (DLS) measures particle size distribution. We fire a laser at the particles in an np dispersion, which scatter light constructively and destructively. The particles are moving through the dispersion by Brownian motion (random movements) and this movement is affected by the size of the particles in the dispersion, with larger particles moving slower than smaller particles. Thus the size of the particles can be measured using the Stokes Einstein equation. Data are taken and averaged for each of the peak means; the z-average value was not used due to it being skewed by larger particle sizes.

The Malvern Zetasizer Nano uses electrophoretic mobility to obtain Zeta-Potential data that helps to understand the stability of dispersions.

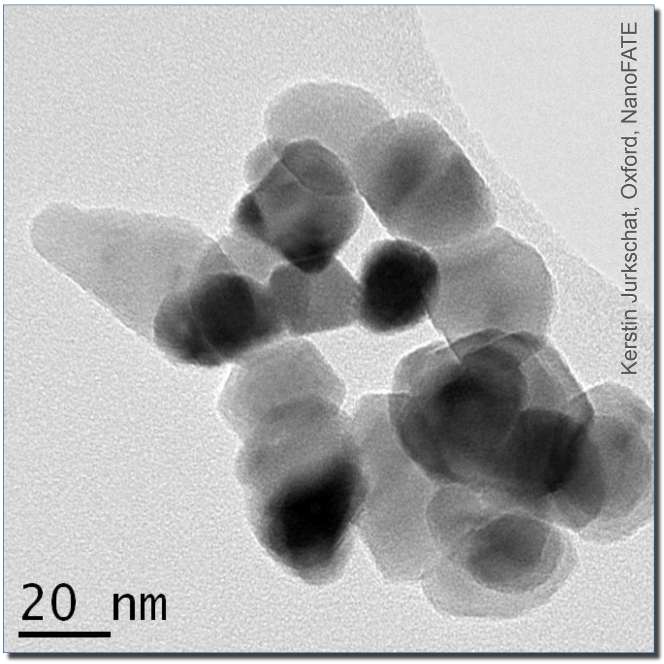
Differential Centrifugation is another technique to assess particle size distribution. Particles settle in a fluid under a gravitational field according to Stokes' law. Sedimentation velocity increases as the square of the particle diameter, so particles that differ in size by only a few percent settle at significantly different rates. In differential sedimentation, all the particles in a sample begin sedimentation as a thin band. The time needed to reach the detector is used to calculate the size of the particles – a mixture of narrow sizes separates into separate and distinct narrow bands, each of which arrives at the detector at a different time. Sizes between 0.005micro and 75 micrometers can be measured; the CPS disc centrifuge can routinely separate particles that differ in size by less than 5%.

Cameron Taylor

University of Oxford Materials Department

TEM uses electrons transmitting through a dried dispersion sample to gain an image of the particles. Size can be estimated visually and compared with the size obtained by DLS, and the shape and agglomeration state can be assessed to give further evidence of what is happening in samples.Dynamic Light Scattering (DLS) to measure particle size distribution. We fire a laser at the particles in an np dispersion, which scatter light constructively and destructively. The particles are moving through the dispersion by Brownian motion (random movements) and this movement is affected by the size of the particles in the dispersion, with larger particles moving slower than smaller particles. Thus the size of the particles can be measured using the Stokes Einstein equation. Data are taken and averaged for each of the peak means; the z-average value was not used due to it being skewed by larger particle sizes.

TEM image



Raman spectroscopy and UV-Vis spectroscopy give insight into composition.

Atomic force microscopy (AFM) will hopefully show how particles directly interact with particular substrates – such as biological samples and soil.

My work will answer the following questions:

- How nanoparticle dispersions change with time: size, shape, dissolution, stability
- How the values obtained by different characterisation methods can be cross-correlated to give a full picture of the particles being studied
- The effect of ultrasonication on particle dispersions
- How nanoparticle dispersions interact with laboratory glassware/soil samples/biological samples.

These questions all fit into NanoFATE Work Package 1 which focuses on the direct interactions between particles, the surrounding media and environmental surfaces. The work package offers fundamental support to the studies carried out throughout the project; for instance, one deliverable is a report on methods, limitations and results for detailed characterisation of “end of test stage” tagged ZnO ENP versions used by experimenters and modellers in WP2, 3, 4 and 5.

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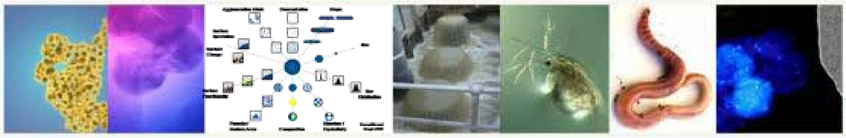

Jacek Wojnarowicz

Solvothermal synthesis of nanocrystalline zinc oxide doped with Co and Gd

Inst. of High Pressure Physics, Polish Academy of Science

Jacek Wojnarowicz graduated from Tadeusz Kościuszko Cracow University of Technology in the field of Chemical Technolology, with a major in Polymer Technology. In his master's thesis, titled 'Polyurethane nanocomposites containing multiferroic ceramics Pb0,94Sr0,06(Zr0,53Ti0,47)0,99Cr0,01O3', he focussed on synthesis and properties of nanocomposites. Currently he is working with Dr Witold Łojkowski at Institute of High Pressure Physics of the Polish Academy of Science on his doctoral thesis, which is dedicated to solvothermal synthesis of nanoparticles.

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In NanoFATE I'm responsible for the synthesis of cobalt and rare earth-doped zinc oxide, and for the functionalisation of nanoparticle surfaces. I'm developing a method of zinc oxide storage via a concentrated suspension and dispersion procedure.

My work involves synthesis and surface modification of nanocrystalline zinc oxide doped with cobalt and gadolinium. I'll undertake investigation of agglomerate size and stability of suspensions obtained with the water used in toxicity tests, and also NP characterisation. Technologies include electron microscopes, surface analyzer, density analyzer, surface tension analyzer, particle size analyzer DLS, particle size analyzer NTA, and X-ray powder diffraction.

My work will answer the following questions:
- *the stability of suspension as function of time*
- *the influence of different water types on agglomerate size and stability.*

The particles are destined for laboratory use by NanoFATE Component 2 partners. I interact with them to know the amount of zinc oxide needed to conduct toxicity studies, what kind of apparatus they may have (e.g. an ultrasonic washer or ultrasonic homogenizer), and the procedure by which they will add commercial ZnO powder to water or soil for toxicity tests.

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