### supported ionic liquid silica nanoparticles are excellent heterogeneous catalysts for the dehydration of fructose to 5-hydroxymethylfurfural

kalpesh sidhpuria, ana daniel-da-silva, tito trindade, joão coutinho

# department of chemistry & CICECO, university of aveiro

Diminishing fossil fuel reserves and growing concerns about global warming have fostered the development of alternative sources of energy and chemicals. Renewable biomass resources are promising alternatives for the sustainable supply of liquid fuels and chemical intermediates. The catalytic conversion of biomass is important to develop alternatives to crude oil derivatives. Among the many biomass-derived chemicals, 5-hydroxymethylfurfural (HMF) is a particularly valuable intermediate for fine chemicals, pharmaceuticals and in biofuel and polymer chemistry. Hence, acid catalyzed dehydration of fructose to HMF has received substantial attention. Homogeneous acid catalyzed processes can achieve only up to 90% fructose conversion with moderate HMF yield, and it has severe drawbacks in terms of equipment corrosion, separation and recycling; while existing heterogeneous acid catalysts can be recycled and have high HMF selectivity, but very low fructose conversion even after a very long reaction time. Consequently, more efficient catalytic systems for the selective production of HMF from fructose need to be developed.

At the University of Aveiro researchers from CICECO have recently developed supported ionic liquid nanoparticles (SILNPs) (Green Chem., 2011, 13, 340-349). The SILNPs are composed of amorphous SiO2, each sample characterized by a distinct average particle size (300 to 600 nm) that depends on the ammonia concentration employed in the synthesis by using a sol-gel method. The silica surfaces have been chemically modified with an ionic liquid via covalent attachment using a silicon alkoxide linker. The SILNPs are a new catalyst that quickly (less than 30 minutes reaction time), and efficiently (99.9% conversion), convert fructose into HMF with yields of 63% in optimized reaction conditions (130°C). These heterogeneous catalysts present improved performances over other zeolites and strong acid ion exchange

resin catalysts previously used, and were shown to be efficiently and easily recycled without any significant loss in fructose conversion and HMF yield. These new catalysts, allowing the conversion of biomass fraction into valuable products, contribute to make the biorefinery dream come true, minimizing our dependency on crude oil derivatives and advancing the world's sustainability.



## direct imaging of Joule heating dynamics and temperature profiling inside a carbon nanotube interconnect

pedro costa<sup>1</sup>, ujjal gautam<sup>2</sup>, yoshio bando<sup>2</sup>, dmitri golberg<sup>2</sup>

 <sup>1</sup> department of ceramics and glass engineering & CICECO, university of aveiro
 <sup>2</sup> national institute for materials science, japan



Resistive heating is a common phenomenon when electronic components are exposed to high current densities. It leads to an accentuated waste of energy and favours electromigration, a frequent cause of circuit failure. Knowing how the building blocks of nanoscaled electronic circuits respond to such electrical stress is essential for their future use in devices. Carbon nanotubes (CNTs) have been widely touted as superior wires to connect the various components of next-generation integrated circuits. Despite almost two decades of intense effort, insight into the internal structural and thermal responses of these structures when subjected to resistive heating has been lacking. On the 9<sup>th</sup> of August 2011, in a report published by Nature Communications (doi: 10.1038/ ncomms1429), Pedro Costa from the University of Aveiro and colleagues from the National Institute for Materials Science, Japan, described how it was possible to directly image the dynamics of Joule heating and extract temperature profiles from the interior of CNTs acting as interconnects.

In general, electrical probing studies of CNTs had been performed in the absence of information concerning its internal structure, with relatively low spatial resolution and often not resolved in time. Consequently, what happened in the tubular channel during the Joule heating process remained a mystery. Working with a transmission electron microscope and an electrical probing sample holder, Costa *et al.* were able to locate the hottest points inside an electrically-heated nanotube due to the solid-to-vapour phase transitions that took place in a carbon-encapsulated semiconductor nanowire. In addition, the team also followed the migration of these hot-spots and their evolution. The sublimation fronts of the confined nanowire acted as temperature markers to understand how heat is distributed along and across the tube.

Besides CNTs, the method reported may be used to evaluate the resistive heating behaviour of other nanoscaled tubular interconnects. Eventually, it may also be envisaged as a test-bed for the study of phase transitions occurring in confined spaces such as nanometer-sized channels of porous materials.

### inversion of the noisy Radon transform on SO(3) by Gabor frames and sparse recovery principles

# paula cerejeiras<sup>1</sup>, milton ferreira<sup>2</sup>, uwe kähler<sup>1</sup>, gerd teschke<sup>3</sup>

<sup>1</sup> department of mathematics & CIDMA, university of aveiro
<sup>2</sup> CIDMA & polytechnic institute of leiria
<sup>3</sup> neubrandenburg university of applied sciences



One of the modern methods in determining the structure of polycristalline materials is the so-called X-ray diffraction tomography. For each incidence ray one measures the diffraction pattern and from this information one desires to determine the crystallographic structure of the material. Mathematically this is done by inverting the so-called spherical Radon transform which is an ill-posed inverse problem. In the paper "Inversion of the noisy Radon transform on SO(3) by Gabor frames and sparse recovery principles", Appl. Comput. Harmon. Anal. (2011) a new method for obtaining a stable approximation of the inverse of the spherical Radon transform was established. X-ray tomography of crystallographic structures using diffraction experiments is a computationally expensive task. To give an idea of the complexity of the problem just by measuring as few as 100 incidence rays and 100 scattered rays one obtains already 10 000 measurements. The developed numerical method reduces the problem greatly by constructing new building blocks (so-called spherical Gabor frames) which allow us to use sparse recovery principles (only a few building blocks have non-zero coefficients) while maintaining a stable approximation of the inverse of the spherical Radon transform. The proposed approach is composed by basic building blocks of the coorbit theory on homogeneous spaces, Gabor frame constructions and variational principles for sparse recovery. The performance of the finally obtained iterative approximation is studied through several experiments and it was shown that this new method works well with noisy data.

Nd isotope composition of marine sediments as a tracer for iceberg provenance in the last glaciation

virgínia martins<sup>1</sup>, josé francisco santos<sup>1</sup>, sara ribeiro<sup>1</sup>, fernando rocha1, andreas mackensen<sup>2</sup>, daniel rey<sup>3</sup>, belén rubio<sup>3</sup>, joão m. alveirinho dias<sup>4</sup>

 <sup>1</sup> department of geosciences & geobiotec, university of aveiro
 <sup>2</sup> alfred wegener institute, germany
 <sup>3</sup> university of vigo, spain
 <sup>4</sup> university of algarve

OMEX core KC 024-19 was studied aiming at to assess the influence of climate changes on the origin and transport of the sediments of the Galician continental slope, in the last 40 thousand years. The sampled sediments are composed mostly of silt and clay, but also include a coarser-grained (sand-sized) fraction, corresponding essentially to foraminifera tests. Another remarkable feature is the occurrence of four depth intervals characterized by abundances greater than usual of relative large terrigenous clasts (considered as ice-rafted debris - IRD), related to melting of massive influxes of icebergs into the North Atlantic during the socalled Heinrich Events (HE). In order to obtain information on the origin of the detrital component of the sediments, 27 selected samples were submitted to a leaching procedure, to eliminate the biogenic fraction, and then analysed for Nd and Sr