

## To.Sc.AI'And: total scattering for nanotechnology in AI'Andalus

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Researchers from 14 different countries *physically* met at the University of Granada (UGR, Spain) for an International Workshop co-organized by UGR and To.Sca.Lab., an experimental and computational laboratory co-founded by the University of Insubria and the Italian National Council of Research (Italy). The scope of this workshop, which followed previous editions held in Como (2015, 2017, and 2019) and in Florianópolis (Brazil, 2018), was introducing innovative wide-angle X-ray total scattering (WAXTS) techniques for the study of nanomaterials, together with complementary small-angle X-ray scattering (SAXS), electron diffraction (ED), and laser scattering (SLS/DLS) methods.

During the last decade, staff researchers of **To.Sca.Lab** (Total Scattering Laboratory, <http://toscalab.uninsubria.it>), a joint laboratory merging experimental and computational aspects and co-founded by the University of Insubria and the Institute of Crystallography of the Italian National Research Council (IC-CNR), have organized several International Summer Schools: first, the "Crystallography for Health and Biosciences" workshop (Masciocchi *et al.*, 2012), followed by many editions of To.Sca.Lake (*Total Scattering for Nanotechnology on the Como Lake*, 2015, 2017, 2019) (Masciocchi *et al.*, 2015, 2017; Bertolotti *et al.*, 2019) and the export of such format to Latin America (*To.Sca.Lat.*), in the 2018 edition, held in Florianópolis in Brazil (Campos *et al.*, 2019).

As evidenced in the scientific programs and in the lists of talks presented during these many years by the different teachers, the *Scattering* techniques based on the use of X-rays (in the wide- and small-angle regions of the reciprocal space, labeled as WAXS and SAXS), often coupled to the usage of X-ray radiation of high brilliance and quality available at synchrotron facilities, have been progressively tied to new experimental and computational methodologies, such as laser scattering, in static (SLS) and dynamic (DLS) modes and, in the 2021 edition, electron diffraction (ED). To these, the crystal chemical/structural analyses supported by the Pair Distribution Function approach (PDF, in 1D and 3D modality that, working in direct space, provides a clear interpretative advantage) were added. All these experimental and modeling aspects constitute the *core* of the scientific activities pursued at the To.Sca.Lab, which aim at: (i) understanding the structure, microstructure, defectiveness, and dynamics of nanoscaled crystalline materials and of partially ordered or disordered species, (ii) characterizing these materials at different levels (from atomic resolution to sub-micrometer sizes), and (iii)

correlating their behavior with their (optical, electronic, thermoelectric, catalytic, etc.) properties.

To the goal of widening the audience of these new approaches to the structural and microstructural characterization of nanosized materials, the 2021 edition of the Workshop, entitled *To.Sc.AI'And: International Workshop On Total Scattering For Nanotechnology In AI'Andalus* (<https://congresos.ugr.es/toscaland/>), was organized as an *in-person* meeting at the Faculty of Sciences of the University of Granada (Spain), with a special focus on an international public of young researchers, post-docs, PhD, and undergraduate students. It was indeed possible thanks to the logistic support of the Granada University and the concomitant health situation, which, during Summer 2021, has seen a rapid descent of the COVID-19 pandemic, particularly in the South of Spain (Andalusia).

The dense scientific program included lessons on scattering techniques, on advanced synthetic methods, and on applications of innovative engineered nanomaterials, with high performances in the energetic, environmental, and biomedical fields. The theoretical talks have been integrated by computational sessions and hands-on tutorials, particularly dedicated to data analysis software programs developed at To.Sca.Lab. (Como, Italy) in strict collaboration with the Paul Scherrer Institute (Villigen, Switzerland) and by Columbia University (New York, USA), coordinated by Simon Billinge. The conference site, the Faculty of Sciences of the University of Granada (Figure 1), is fully appropriate for a (deliberately limited) participation, fixed at 40 attendees (plus speakers), both for obvious sanitary reasons and for making the tutorial sessions and the computational laboratory easy to manage and of high effectiveness. Invited speakers at To.Sc.AI'And were internationally known experts in the field of scattering methods and in the preparation and characterization of organic and inorganic nanoparticles.

This Workshop began with the delivery of three lectures on X-ray scattering techniques. Hans-Beat Bürgi (University of Bern) gave a brilliant overview on the measure and interpretation of diffuse scattering in ionic and molecular crystals, with a special emphasis on correlated defectiveness. Federica Bertolotti (Università dell'Insubria and To.Sca.Lab) has presented the basics of diffraction methods for micrometer- and nanometer-sized powders, highlighting the difference between conventional Bragg and non-Bragg approaches. Finally, Antonella Guagliardi (IC-CNR and To.Sca.Lab) illustrated theoretical aspects of radiation-matter





Figure 1. The massive entrance at the Faculty of Sciences of the Granada University where To.Sc.al'And was held.

interaction, and the rigorous derivation of the Debye scattering equation (Debye, 1915), valid for isotropic systems, such as liquids, colloidal suspensions, and nanopowders with random orientation.

In the afternoon, Antonio Cervellino (Paul Scherrer Institute) performed a series of experimental measures through a *remote* connection to the Material Science Beamline of the Swiss Light Source using a robot capable of mounting and dismounting samples loaded in sealed capillaries and collecting scattering data from standard reference polycrystalline samples and from defective nanoscaled materials. The session was eventually completed with the first of the two lectures offered by Simon Billinge, where the theory, and, in the following day, the applications of the PDF method to the study of nanomaterials were presented.

In the second day, an intriguing journey to the organic nanoparticles' World for biomedical applications was illustrated by Nora Ventosa (ICMAB-CSIC), followed by the lecture of Jan Skov Pedersen (Aarhus University), who presented the theory of small-angle scattering methods of analysis and their application in the material science and soft matter fields.

In the afternoon, an additional talk by Hans-Beat Bürgi on innovative approaches to 3D-PDF preceded the captivating presentation by Tatiana Gorelik (University of Ulm) on the capability of electron diffraction methods, starting from newly designed instruments to applications in diverse fields of nanosized material, encompassing organics, inorganic, and hybrid species.

The third day of the Workshop was entirely dedicated to tutorial and *hands-on* sessions on X-ray total scattering programs, operating in the reciprocal and real space, using the Debussy (Cervellino *et al.*, 2015) and PdfGui (Farrow *et al.*, 2007) software.

On the following day, the lecture of Daniel Maspoch (ICN2, Barcelona) focused on hybrid inorganic–organic materials and on their time evolution, mostly morphological and chemically induced. Next, Antonella Guagliardi presented several case studies of the *Debye Function Analysis*, taken from the recent scientific literature, with a specific emphasis on different classes of *quantum dots* for optical and photovoltaic applications. The afternoon session was dedicated to short presentations delivered by the young participants at To.Sc. Al'And. These talks included, in a non-exhaustive list, studies on inorganic nanomaterials, MOFs (MOFs = Metal Organic Frameworks), biological systems, and engineered species with luminescent and magnetic properties.

Just before the closure of the Workshop, Fabio Ferri (Università dell'Insubria and To.Sca.Lab) presented (laser-generated) visible light scattering techniques, in static and dynamic modes, highlighting both theoretical and experimental aspects and applications to sub-micrometric materials. The realization of a previously recorded video, illustrating instrumental details, jointly with data analysis procedures of a laser light-scattering experiment on colloidal suspension, enabled the entire audience to observe, and comment in real time on those numerical and experimental aspects that a simple *ex-cathedra* lecture cannot convey. Finally, José Manuel Delgado López (University of Granada) illustrated structural and morphological aspects of biomimetic samples of biomedical interest (nanoapatites, collagen) and of “green”

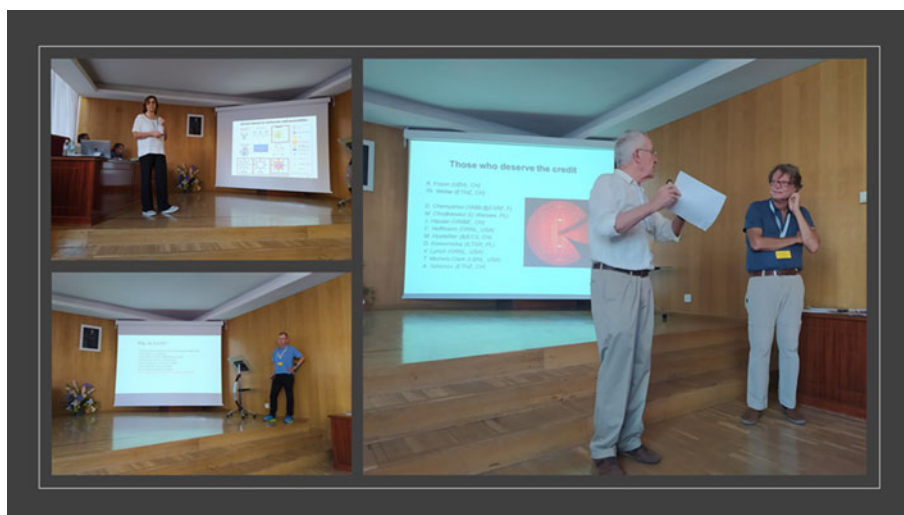


Figure 2. Snapshots from some scientific presentations. Anticlockwise from top left, Nora Ventosa, Jan Skov Pedersen, Hans Beat Bürgi, and Norberto Masciocchi.



Figure 3. A glance on the rich scientific/cultural *full-immersion* program of To.Sc.Al'And in Granada, including a picture of some of the speakers relaxing in the sea of Salobreña after the school closure.



Figure 4. The ICDD-sponsored award ceremony for young foreign attendees. On the left, the chairs of the school: Norberto Masciocchi, Antonella Guagliardi, and Jorge Navarro.

nanofertilizers prepared within the HYPATIA project (calcium phosphates modified by nitrogen-rich exogenous sources – nitrates and urea). **Figure 2** portrays some of the various, and diverse, moments of the scientific presentations.

As witnessed from further images in **Figure 3**, the hospitality of the University of Granada enabled, simultaneously,

the intense work of speakers and attendees, and the fruitful sharing of expertise, problems, and scientific and cultural motivations in a real context of “full immersion”.

During the entire Workshop duration, five technical/scientific presentations were offered by Detlef Beckers (Malvern Panalytical, NL) and Michael Evans (Bruker, DE)



on new instrumental solutions for X-rays total scattering applications in the laboratory; Gustavo Santiso Quiñones (Eldico, CH) and Partha Das (Nanomegas, BE) on recent developments of electron diffraction techniques, and Christian Schürmann (Rigaku Europe, DE) who presented new multi-functional diffraction instrumentation.

Needless to say, organizing and realizing this event would not have been possible without the help of several public bodies and private companies, here listed in a non-ordered manner: International Union of Crystallography (IUCr), European Crystallography Association (ECA), International Center for Diffraction Data (ICDD), Associazione Italiana di Cristallografia (AIC), Real Sociedad Española de Química (RSEQ - GE3C) and, as generous commercial sponsors, Bruker, Malvern Panalytical, Rigaku, Eldico, Nanomegas, Dectris, Excelsus, and Nanomaterials@MDPI. Their substantial economic support enabled the presence in Granada of several foreign attendees from different European countries. Gender equality was also ensured both in the list of speakers and particularly in the list of attendees, 48% of whom were young ladies. [Figure 4](#) portrays one group of awardees (here, those sponsored by ICDD). Last, but not least, we would like to highlight the fundamental assistance and help by young *granaínos* (Francisco J. Carmona, José Manuel Delgado López, and Rebecca Vismara, coordinated by Jorge A.R. Navarro) and the administrative help of Mr. Antonio de la Torre. To all of them, we are heartily indebted for the economical, logistic, and scientific support which fostered the great success of this first *in person* post-Covid event. We also acknowledge partial financial support by MIUR - Project HY-TEC, PRIN 2017L8WW48.

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