

Report on the To.Sca.Lake 2.0 Workshop, Total Scattering for Nanotechnology on the Como Lake

Norberto Masciocchi, Fabio Ferri

Dipartimento di Scienza e Alta Tecnologia and To.Sca.Lab, Università dell'Insubria, via Valleggio 11, 22100 Como (Italy)

Federica Bertolotti

Aarhus Institute of Advanced Studies (AIAS), Aarhus University, Høegh-Guldbergs Gade 6B, 8000 Aarhus C (Denmark)

Antonietta Guagliardi

Istituto di Cristallografia and To.Sca.Lab, Consiglio Nazionale delle Ricerche, via Valleggio 11, 22100 Como (Italy)

Summary

In the frame of the activities sponsored by the Lake Como School of Advanced Studies, in late May 2017 more than 80 participants (including nearly 60 students, post-docs and young researchers) from about 20 different European, North and South American and Asian Countries gathered in Como, Italy, for an International Workshop co-organized by the University of Insubria and the Institute of Crystallography of the Italian National Research Council. Scope of this workshop was introducing innovative wide angle X-ray total scattering techniques (WAXTS) for the study of nanocrystalline materials, based either on the Pair Distribution Function approach or on the Debye scattering equation. Their complementary nature with small-angle X-ray (SAXS) and static/dynamic light (LS) scattering was additionally discussed. Lectures on scattering theory and on experimental and computational aspects were supplemented by a few presentations focusing on the synthesis and applications of advanced organic, inorganic and hybrid nanomaterials. Demo and hands-on tutorial sessions on the well renowned PDFgui and Debussy Suites, as well as short presentations by the attendees, were organized. This brief account highlights the topics discussed during the meeting.

Highly advanced courses in topical fields are not typically provided in Academy and often require the specific organization of events specifically tailored to Ph.D. students, postdocs or young researchers on the verge of their scientific careers. Joining the efforts of the Lake Como School for Advanced Studies, and those of scientists from the University of Insubria and the Crystallography Institute of the Italian National Council of Research (IC-CNR), a successful Summer School was organized in Como at the beautiful location of the 18th Century Villa del Grumello (see Figure 1) in late May 2017. This event, labeled “*To.Sca.Lake 2.0: Total Scattering for Nanotechnology on the Como Lake 2.0*”, follows the first edition of To.Sca.Lake (Masciocchi, Bertolotti and Guagliardi, 2015), by nearly doubling the number of participants, whilst adding some new topics and sessions to the scientific program. Figure 2 portrays the group photo.

The organization of these activities falls well within the educational section of the **To.Sca.Lab** project (see also toscalab.uninsubria.it). Indeed, in the intentions of the founders of To.Sca.Lab (a Total Scattering Laboratory co-founded in 2013 by University of Insubria and the Institute of Crystallography of the Italian CNR), theoretical and experimental expertise in chemistry, crystallography and physics are merged within a unifying project based on *Scattering Techniques* (from X-rays to Visible Light). Specifically, To.Sca.Lab scientific activities aim at reconstructing structural, microstructural and dynamic behavior of nanocrystalline, partially ordered and disordered materials at different length scales (ranging from atomic resolution to the mm size), and to correlate it with materials functional properties.

In order to widen the scientific topics pertinent to the To.Sca.Lab project and already discussed in the first To.Sca.Lake School (Masciocchi, Bertolotti and Guagliardi, 2015), the 2017 event included several talks on single-crystal diffuse scattering, 1D and 3D Pair Distribution Function analyses and sessions dedicated to the daily scientific activities of the young participants. As lecturers of To.Sca.Lake 2.0, world renowned experts in the field of scattering methods, in the preparation and characterization of inorganic and organic nanoparticles, were invited.

In the first day, three introductory presentations on X-ray scattering techniques were delivered. Hans-Beat Bürgi (University of Bern and Zurich, Switzerland) brilliantly presented the basics of diffuse scattering measurement and its interpretation in ionic and molecular crystals, with particular emphasis on correlated defectiveness. Quantum crystallography methods were also introduced. Norberto Masciocchi (University of Insubria and To.Sca.Lab, Italy) presented the basics of the powder diffraction methods, highlighting the occurrence of (highly informative) subtle

anomalies and the differences between the Bragg and non-Bragg scattering approaches. Finally, Antonio Cervellino (Paul Scherrer Institut, Switzerland) introduced a few aspects of radiation-matter interaction, and the rigorous derivation of the Debye scattering equation (DSE, Debye, 1915), valid for isotropic systems, such as liquids, colloidal suspensions and randomly oriented powders. Experimental aspects for obtaining the “best” total scattering traces at a synchrotron source were also discussed.

In the following day, Simon Billinge (Columbia University, New York, USA) presented the theoretical basis of the 1D Pair Distribution Function (PDF) approach, together with some technical aspects and some advanced scientific results obtained in the field of inorganic nanoparticles and in organic (molecular) materials of industrial interest. Few forefront applications of PDF computed tomography on Pd/PdO catalysts and batteries were also presented. This lecture was followed by Antonella Guagliardi's (Institute of Crystallography- CNR and To.Sca.Lab, Italy) fascinating presentation on the innovative Debye Function Analysis implemented in the highly performing Debussy Suite of programs (Cervellino, Guagliardi, Giannini, 2010; Cervellino, Frison, Bertolotti, Guagliardi, 2015). Recent applications in the field of inorganic and hybrid quantum dots characterization in the solid and colloidal state were also illustrated (Bertolotti et al., 2016; 2017).

On the third day, Maksym Kovalenko (ETH Zurich, Switzerland) delivered a mesmerizing presentation on the field of nanosized perovskites of high technological interest in photovoltaics, light emitting and γ -rays detection devices, and energy storage fields. Their synthesis, characterization, structural aspects and implementation into innovative devices were deeply discussed. Hans-Beat Bürgi (University of Bern and Zurich, Switzerland) gave another interesting talk, where 3D Pair Distribution Functions and deviations from ideality made it possible to determine the correct structural models for technologically relevant up-conversion materials, such as sodium fluorolanthanides.

On the next day, Nora Ventosa (ICMAB-CSIC, Spain) delivered a presentation on organic nanomaterials, illustrating the rich world of micelles, liposomes and quatsomes, and their innovative applications in nanomedicine. Later, Jan Skov Pedersen (University of Aarhus, Denmark) showed the power of small-angle X-ray scattering (SAXS) technique in biosciences and, with recent examples from the literature, in characterizing colloids or powders of inorganic nanomaterials. His lecture was followed by a talk by Fabio Ferri (University of Insubria and To.Sca.Lab, Italy), focusing

on visible light scattering techniques, in static and dynamic mode, with emphasis on the theoretical aspects and applications to sub-micrometer-sized materials.

Tutorial sessions were also presented, with attendees working on their laptops with the PDFGui (Farrow et al., 2007) and Debussy (Cervellino et al., 2015) software to extract useful structural and microstructural information from total scattering data collected at dedicated BNL (Brookhaven National Laboratory) and SLS (Swiss Light Source) beamlines. The teachers [Simon Billinge and Maxwell Terban (Columbia University, USA), and the entire Debussy Team – Antonella Guagliardi (Como, IT), Federica Bertolotti (Aarhus, CH), Ruggero Frison (Zurich, CH) and Antonio Cervellino (PSI, CH)] did an excellent job in showing most features of both PDF and DSE approaches to the very interested audience. A computational Demo session was also provided by an additional talk by Jan Skov Pedersen (University of Aarhus, DK), while, on the last day, a live DLS experiment with subsequent data treatment, was organized by Fabio Ferri (University of Insubria and To.Sca.Lab, IT), who showed the benefits (and the pitfalls) of DLS analysis.

Additionally, four technical presentations were also proposed by Geert Vanhoyland (Bruker, Germany), Marco Sommariva (Panalytical, The Netherlands), Jürgen Grässlin (Rigaku, Japan) and Alexander Pilcher (Anton Paar, Austria), all raising a wide interest in the young audience. Finally, two sessions dedicated to short presentation by the young attendees were organized, with nearly twenty presentations of the highest levels; motivations for participation in this Summer School clearly emerged, most talks immediately fostering scientific contacts among the participants. The geographical origin of all attendees is shown in Figure 3.

Of course, this event could not have existed without the help of several public bodies and private companies, here collectively gathered in a non-ordered list: Lake Como School for Advanced Studies, To.Sca.Lab., University of Insubria, IC-CNR, the Italian Crystallographic Association, the International Union of Crystallography, the International Center for Diffraction Data and, as generous commercial sponsors, Bruker, Panalytical, Assing/Rigaku, Anton Paar and Excelsus. The patronage by INSTM (Istituto Nazionale per la Scienza e Tecnologia dei Materiali) was also offered. We are heartily indebted to all of them for their financial support.

As things can't be expected to turn out right every time, we need to add a sad remark. Despite fully adopting "IUCr Scientific Freedom Policy Statement": *The Organizing Committee of the To.Sca.Lake 2.0 shall observe the basic policy of non-discrimination and affirms the right and freedom of scientists to associate in international scientific activity without regard to such factors*

as ethnic origin, religion, citizenship, language, political stance, gender, sex or age, in accordance with the Statutes of the International Council for Science. At this meeting, no barriers will exist which would prevent the participation of bona fide scientists, we faced unexpected difficulties in obtaining the Visa to enter Italy for a couple of attendees: Zhaled Ebrahimejad from Alzahra University of Tehran (Iran) and Nzikahyel Simon from the University of Uyo (Nigeria), to whom this report is dedicated.

Use of IUCr Funds:

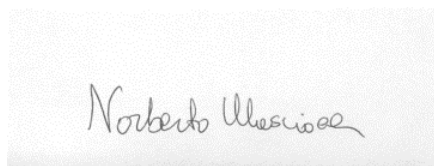
IUCr generously provided 3000,00 US\$, converted to ca. 2730,00 Euros. They have been used to support Young Scientists from Ukraine, India, Brazil and Argentina.

Name of meeting: **To.Sca.Lake 2.0 Workshop, Total Scattering for Nanotechnology on the Como Lake**
Location: **Villa del Grumello, Como (Italy)**
Date: **May 29th, 2017 – June 2nd, 2017**

Name	PhD student, Post doc or other (please indicate)	Age	Address	Email address	Amount awarded (Euro)
Rodrigo Uchida Ichikawa	PhD student	28	Inst. De Pesquisas Energeticas e Nucleares, Sao Paulo, Brasil	ichikawa@usp.br	1130.30
Pradeep Shambogh	Post-doc	30	Poornaprajna Institute of Scientific Research (PPISR), Bangalore, India	pradeep.shanbogh@gmail.com	866.00
Fernando Pomiro	Post-doc	30	Instituto de Física del Litoral, Santa Fe, Argentina	fernando.pomiro@santafe-conicet.gov.ar	640.00
Oleksiy Konotop	PhD student	30	National Academy of Sciences of Ukraine , Kharkiv, Ukraine	konotop@ilt.kharkov.ua	200.00
			Total (Euro)		2836.30
			Amount received from IUCr (Euro)	3000,00 USD	Ca. 2730
			Difference (USD)	Compensated by other funds	Ca.120

Note: Funds for young scientists should be used solely for travel and subsistence and **not** as a waiver for the registration fee. FUNDS FOR YOUNG SCIENTISTS HAVE BEEN USED UNIQUELY FOR FLIGHT TICKETS AND ACCOMMODATION IN SHARED ROOMS IN TOWN.

Signature



Date 16.06.2017

Figures



Figure 1. The conference venue, the 18th Century Villa del Grumello, facing the Como Lake.



Figure 2. The group photo of the To.Sca.Lake Workshop. In the inset, the To.Sca.Lab logo.

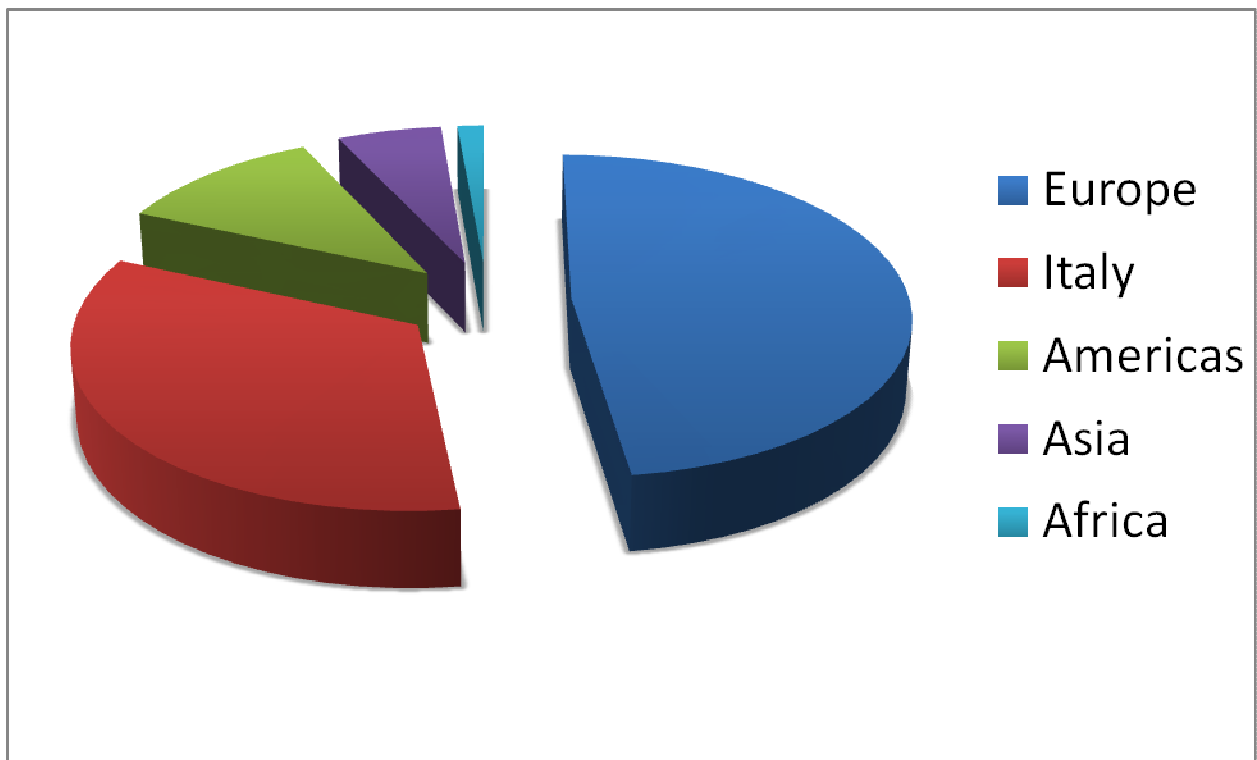


Figure 3. Geographical Origin of Attendees.

REFERENCES

Federica Bertolotti, Dmitry N. Dirin, Maria Ibáñez, Frank Krumeich, Antonio Cervellino, Ruggero Frison, Oleksandr Voznyy, Edward H. Sargent, Maksym V. Kovalenko, Antonietta Guagliardi, Norberto Masciocchi, Crystal symmetry breaking and vacancies in colloidal lead chalcogenide quantum dots. *Nature Mater.*, 15 (2016), 987-994.

Federica Bertolotti, Loredana Protesescu, Maksym V. Kovalenko, Sergey Yakunin, Antonio Cervellino, Simon J.L. Billinge, Maxwell W. Terban, Jan S. Pedersen, Norberto Masciocchi, Antonietta Guagliardi, Coherent Nanotwins and Dynamic Disorder in Cesium Lead Halide Perovskite Nanocrystals, *ACS Nano* 11 (2017) 3819-3831.

Antonio Cervellino, Cinzia Giannini, Antonietta Guagliardi, DEBUSSY: a Debye user system for nanocrystalline materials, 43 (2010) 1543-1547.

Antonio Cervellino, Ruggero Frison, Federica Bertolotti, Antonietta Guagliardi, DEBUSSY 2.0 - the new release of a Debye User System for nanocrystalline and/or disordered materials, *J. Appl. Crystallogr.* 48 (2015) 2026-2032.

Peter Debye, Zerstreung von Röntgenstrahlen, *Ann. Phys.* 351 (1915) 809–823.

Christopher L. Farrow, Pavol Juhás, Jiwu Liu, Dmitriy Bryndin, Emil S. Božin, Jacques Bloch, Thomas Proffen, Simon J. L. Billinge, PDFfit2 and PDFgui: computer programs for studying nanostructure in crystals, *J. Phys.: Condens. Mat.*, 19 (2007) 335219.

Norberto Masciocchi, Federica Bertolotti and Antonietta Guagliardi, Report on the To.Sca.Lake Workshop, Total Scattering for Nanotechnology held at Como Lake, *Powder Diffr.*, 30 (2015) 320-322.