



## Angela Altomare

### Personal Details

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Nationality: Italian  
D.O.B.: 16.08.1963

### Education

*University of Bari, Bari (Italy), Graduated October 1988*

- Degree in Physics (general address)
- Thesis: ‘Su un modello di quarks confinati con simmetria chirale approssimata (On a model of confined quarks with approximate chiral symmetry)’.
  - Received a mark of 110/110 *cum laude*

*Liceo Scientifico, Molfetta (Bari), Italy, Graduated 1982*

- Received Scientific Diploma, with a mark of 60/60

### Research Experience

*Scientific responsible of the research team involved in the following scientific objectives: structural characterization by single crystal and microcrystalline powder diffraction data; developing innovative methods aimed at structural solution from single crystal and powder diffraction data; qualitative and quantitative analysis of multiphase mixtures by powder diffraction; development of new computational algorithms and their implementation in crystallographic software (in particular for the characterization of powders); management of the laboratory for microcrystalline powder diffractometry, January 2009 – present*

*CNR (National Research Council of Italy) Research Director, IC (Institute of Crystallography)-CNR, Bari (Italy), December 2021 – present*

*CNR Senior Researcher, IC-CNR, Bari (Italy), December 2001 – 2021*

*CNR Researcher, IRMEC (Institute for the Development of Crystallographic Methodologies)-CNR, Bari (Italy), February 2001 – December 2001*

*CNR Researcher, IRMEC-CNR, July 1999 – February 2001*

- Hired to work with Prof. C. Giacovazzo, Full Ordinary Professor of Mineralogy at the University of Bari
- Works in the following fields:
  - Optimization of the extraction procedures and analysis of the integrated intensities from a powder experimental diffraction pattern;
  - Structural refinement with powder data;
  - Quantitative Analysis from powder diffraction;
  - High-temperature powder diffraction by using a rotating anode and a curved detector CPS120.

*Visiting scientist in the laboratory of Prof. Daniel Louer, University of Rennes, France, in the frame of the CNR International Exchange Program, February 5 – 24, 1996*

- Making experience with an X-ray diffractometer equipped with a CPS detector (Curved Position Sensitive) 120° curved.

*Person in charge of the diffraction laboratory, IRMEC-CNR, December 1996 – June 2001*

*CNR Researcher, IRMEC-CNR, July 1994 – July 1999*

- Appointed by Prof. C. Giacobozzo
- Works on the following research projects:
  - Decomposition of powder X-ray diffraction profiles
  - Automatic refinement of powder structures
  - Quantitative Analysis from powder diffraction
  - High pressure and high temperature powder diffraction.

*CNR Researcher, IRMEC-CNR, June 1989 – June 1994*

- Tackles the main problems of the structure solution by using diffraction data from both single crystal and powders.

*Collaboration with Prof. Carmelo Giacobozzo, December 1988 – June 1989*

- Works on:
  - The solution of the phase problem in crystallography
  - Elaboration of new software
  - The development of new crystallographic methodologies.

## **Research Projects**

*She works on the following projects:*

*Associated Investigator of the project PRIN-MIUR (acronym for Research Projects of significant National Interest- Ministry of Education, University and Research) Research Project, Bando 2017, October 2019-present.*

- Title of the research: ‘Unlocking Sustainable Technologies Through Nature-Inspired Solvents - (NATUREChem)’.

*Fondo per la Crescita Sostenibile - Bando "HORIZON 2020" PON (acronym for National Operative Program) I&C Research Project, July 2017 – May 2021*

- Title of the project: ‘Studio, progettazione e prototipazione di un kit innovativo per la diagnosi precoce e non invasiva della celiachia mediante marcatori genetici’.

*Bilateral agreement CNR/MOES (Albania), June 2018 – December 2020*

- Title of the research: ‘New nanomaterials for applications in conservation and consolidation of stony materials part of Culture Heritage in Albania’.

*Person in charge of the CNR Activity project (Research Group), January 2016 – present*

- Title of the research: ‘EXPO2015’

*Proponent of the financed CNR project 'Short-Term Mobility 2016', 4 July 2016-15 July 2016*

- This allowed Dr. Martina Vrankic of ‘Ruder Boskovic Institute’, division of Materials Physics in Zagreb, Croatia, a scientific 10 days visit at IC-CNR of Bari.

*Person in charge of the 'Software and know how license' contract between the CNR ‘Dipartimento di Scienze Chimiche e Tecnologie dei Materiali’ and RIGAKU Corporation, 19 October 2015-01 October 2018 automatically renewed for other three years.*

- This regards payment of royalty from RIGAKU to IC-CNR for each non-exclusive license for each sale by RIGAKU, of the software EXPO2015, developed by the research group coordinated by Dr. Altomare.

*Proponent of the scientific project funded 'Short-Term Mobility 2013', 30 September 2013-11 October 2013*

- This allowed Dr. Igor Derd of 'Ruder Boskovic Institute', division of Materials Physics in Zagreb, Croatia, a scientific 10 days visit at the Institute of Crystallography (IC) -CNR of Bari.

*FIRB (acronym for Future in Research) Research Project, February 2012–February 2016*

- Title of the project: 'Rete Integrata per la Nano Medicina (RINAME) (Integrated network for Nano Medicine) (RINAME)'.

*PON Research Project, July 2011 – October 2015*

- Title of the project: 'IT@CHA-Tecnologie Italiane per applicazioni avanzate nei Beni Culturali (IT@CHA-Italian Technologies for Advanced application in Cultural Heritage Assets)'.

*FIRB Research Project, December 2010–June 2014*

- Title of the project: 'Microtecnologie e moderne tecniche spettroscopiche e diffrattometriche per lo sviluppo e la razionalizzazione dei processi di sintesi stereoselettivi ecosostenibili (Microtechnology and modern diffraction and spectroscopic techniques for the development and streamlining of sustainable stereoselective synthesis processes)'.

*Proponent of the scientific project funded 'Short-Term Mobility 2010', 13 September 2010-24 September 2010*

- This allowed Dr. Jasminka Popovic of 'Ruder Boskovic Institute', division of Materials Physics in Zagreb, Croatia, a scientific 10 days visit at the Institute of Crystallography (IC) -CNR of Bari.

*Person in charge of the CNR Departmental project (Research Group) (ex CNR-PM.P01.024 task or Commessa-CNR), January 2009 – present*

- Title of the research: 'Metodologie Cristallografiche: sviluppo e applicazione a materiali di varia complessità (Crystallographic methodologies: development and application to materials of varying complexity)'.

*Person in charge of the CNR project (RSTL), January 2008 – December 2010*

- Title of the research: 'Metodologie Innovative per la soluzione strutturale da materiali policristallini (Innovative Methodologies for the structure solution from polycrystalline materials)'.

*Person in charge of the project PRIN-MIUR Research Project, September 2008 – November 2010*

- Title of the research: 'Applicazioni delle tecniche MAD e Sviluppo di nuovi algoritmi di calcolo per migliorare il processo di risoluzione delle strutture cristalline attraverso i dati di diffrazione da polveri (Applications of MAD techniques and Development of new computing algorithms to improve the process of crystal structure solution by powder diffraction data)'.

*Person in charge of commercial license agreement between IC-CNR and companies interested in the EXPO software, 2005 – 2015*

*MIUR (acronym for Ministry of Education, University and Research) Research Project, May 2004 – October 2007*

- Title of the research: 'Global Phasing: dalle polveri alle Macromolecole (Global Phasing: from powders to Macromolecules)'.

*MIUR Research Project, September 2002 – September 2006*

- Title of the research: 'TECSIS: Tecnologie Diagnostiche e sistemi intelligenti per lo sviluppo di parchi archeologici del Sud d'Italia (TECSIS: Diagnostic technologies and intelligent systems for the development of archaeological parks of Southern Italy)'.

*CNR Research Project for Cultural Heritage, January 1996 – December 2000*

- Title of the research: ‘Analisi quantitativa da dati diffrattometrici: sviluppo di metodi e realizzazione di un programma di calcolo (Quantitative Analysis by Diffraction Data: Development of Methods and Realization of a Computing Program) ’.

## **Lectures**

*Invited speaker, Online Event RIGAKU XRD FORUM Powder Diffraction (<https://www.rigaku.com/forum/xrd2021/program.php>), March 2-4, 2021*

- Lecture: ‘Progress in structure solution using powder diffraction data. The software EXPO’

*Invited speaker, The 2nd International Online Conference on Crystals ([https://sciforum.net/conference/IOCC\\_2020](https://sciforum.net/conference/IOCC_2020)), November 10-20, 2020*

- Lecture: ‘Polycrystalline Materials: Crystal Structure Solution in the Reciprocal Space or/and Direct Space?’

*Invited speaker, Online Seminar, Chemistry Department, Lancaster University (UK), June 29, 2020*

- Lecture: ‘EXPO: advanced software for solving crystal structure by powder diffraction data’

*Invited Lecturer & Tutor, EXPO&more International Workshop, organized by IC-CNR, Bari (Italy), September 30-October 3, 2019*

- Lecture: ‘The structure solution process in the EXPO software’.
- Lecture: ‘Structure model optimization’

*Scientific Representative of Visiting Scientists from Algeria to IC-CNR, Bari (Italy), February 8-13, 2019*

*Invited speaker as Recipient of Mario Mammi AIC (Italian Crystallographic Association) Award, Fifth Meeting of the Italian and Spanish Crystallographic Associations (MISCA V), Naples (Italy), September 4-7, 2019*

- Lecture: ‘Development and application of crystallographic methodologies for powder diffraction’

*Esteemed lecturer, Rudjer Bošković Institute, Zagreb (Italy), Croatia, November 27-30, 2018*

- Lecture: ‘Crystal structure solution by powder diffraction data: methods, software, applications’

*Invited speaker, 3rd Joint AIC (Italian Crystallographic Association)-SILS (Italian Synchrotron Radiation Society) Conference, Rome (Italy), June 25-28, 2018*

- Lecture: ‘Advanced methods for solving crystal structure by powder diffraction data’

*Invited speaker, 2° Workshop organized by the ‘Instrumentation and Calculation Commission’ of the Italian Crystallographic Association (Title ‘L’esperienza flessibile: studi di diffrazione in condizioni non ambientali’), Bari (Italy), February 22, 2017*

- Lecture: ‘Concetti base della diffrazione X da polveri’

*Invited speaker, Associazione Italiana di Cristallografia 50 anni e non li dimostra - 1967-2017, celebrating meeting organized by Italian Crystallographic Association, Rome (Italy), January 19, 2017*

- Lecture: ‘Le Metodologie Cristallografiche tra Presente e Futuro’

*Scientific Representative of Visiting Scientists from Algeria to IC-CNR, Bari, Italy, June 1-12, 2015*

*Invited speaker, CBGA One Day Workshop on Crystallography, Tirana (Albania), September 25, 2014*

- Lecture: ‘Powder X-ray diffraction: theory and applications’

*Invited speaker, European Materials Research Society 2014 Fall Meeting, Symposium ‘Crystallography in materials science: novel methods for novel materials’, Warsaw (Poland), September 15-18, 2014*

- Lecture: ‘Recent advances in crystal structure solution by powder diffraction data’

*Invited Lecturer & Tutor, International EXPO/SIR Workshop organized by IC-CNR, Bari (Italy), April 10-13, 2014*

*Plenary lecturer, 22<sup>nd</sup> Croatian-Slovenian Crystallographic Meeting, Biograd (Croatia), June 12-16, 2013*

- Lecture: 'The Challenge of the Ab-initio Crystal Structure Solution by Powder Diffraction Data: the EXPO Software'

*Invited speaker, European Powder Diffraction Conference EPDIC13, Grenoble (France), October 28-31, 2012*

- Lecture: 'The new COVMAP method in the EXPO package'

*Invited speaker, XXII Congress and General Assembly of the International Union of Crystallography (IUCr), Madrid (Spain), August 22-30, 2011*

- Lecture: 'The Automation and efficiency in the powder structure solution by EXPO package'.

*Invited speaker, 12<sup>th</sup> European Powder Diffraction Conference, Darmstadt (Germany), August 27-30, 2010*

- Lecture: 'The DUAL-SPACE resolution bias correction procedure in EXPO2010'.

*Invited speaker, XXV European Crystallographic Meeting, Istanbul (Turkey), August 16-21, 2009*

- Lecture: 'Minimally resolution biased electron-density maps'.

*Invited Lecturer & Tutor, International workshop 'PHARE 2009 A modular workshop on global PHase REtrieval (Module 1- Crystal structure solution and refinement from powder data)' organized by IC-CNR, Martina Franca (Italy), April 15-17, 2009*

*Invited speaker, 8<sup>th</sup> Pharmaceutical Powder X-ray Diffraction Symposium & Workshop organized by 'The International Centre for Diffraction Data', Glasgow (Scotland), May 4-7, 2009*

- Lecture: 'Advances in crystal structure solution by EXPO2008'.

*Invited speaker, XXXV Meeting of the Italian Crystallographic Association (AIC), Ferrara (Italy), September 18-21, 2006*

- Lecture: 'Structure solution by powder diffraction with Expo2006: the state of the art and the future'.

*Invited Lecturer & Tutor, Departamento de Física Fundamental II, Universidad de La Laguna Tenerife, Spain, December 12-16, 2006*

- Invited by Dr. Javier Gonzalez-Platas to hold a seminar on 'Ab Initio Structure Solution by powder diffraction data with EXPO2006' and realized the workshop 'EXPO2006 in action'.

*Speaker, XXXIV Meeting of the Italian Crystallographic Association (AIC), Roma (Italy), September 26-29, 2004*

- Lecture: 'EXPO2004: from powder diffraction pattern to structure solution'.

*Invited speaker, 19<sup>th</sup> International Congress of Crystallography, Geneva (Switzerland), August 6-15, 2002*

- Lecture: 'A new method for completing a polyhedrally coordinated structure in EXPO2002'.

*Invited speaker, National Institute of Standards & Technology (NIST), Gaithersburg, Maryland (USA), April 22-25, 2001*

- Lecture: 'Direct Methods Optimised for Solving Crystal Structure by Powder Diffraction Data: Limits, Strategies, and Prospects'.

*Speaker, 12th European Powder Diffraction Conference, Nancy (France), August 25-31, 2000*

- Lecture: "Monte Carlo techniques in EXPO".

*Speaker, Fifth European Powder Diffraction Conference EPDIC-5, Parma (Italy), May 25-28 1997*

- Lecture: 'Expo: from the powder pattern to the crystal structure'.

*Invited Lecturer & Tutor, V SIR Workshop 'SIRWARE96: Single Crystal and Powder Data X-Rays, neutrons and electrons', international workshop organized by IRMEC-CNR, Bari (Italy), December 17-20, 1996*

- Lecture: 'EXTRA: how to extract  $|F|$  from powder patterns' 'Pseudo – Translational Symmetry'
- Lecture: 'Pseudo – Translational Symmetry'.

*Invited Lecturer & Tutor, Chemical Department, University of Aarhus (Denmark), October 1-8, 1993*

- Invited by Prof. A.N. Christensen to participate in a class on the application of Direct Methods programs SIR92 and SIRPOW.92.

*Invited Lecturer & Tutor, IV SIR Workshop: 'SIR92-SIRPOW.92: two powerful tools for solving crystal structure via single crystal and powder data', international workshop organized by IRMEC-CNR, Bari (Italy), April 5-7, 1993*

*Speaker, XXII Meeting of the Italian Crystallographic Association (AIC), L'Aquila (Italy), October 14-16, 1992*

- Lecture: 'Il SIRPOW.92: un package per la risoluzione strutturale da dati da polveri'.

*Speaker, Fourteenth European Crystallographic Meeting ECM-14, Enschede (the Netherlands), August 2-7 1992*

- Lecture: 'About the least-squares refinement of a molecular model via powder data'.

## **Chairing Sessions**

*33<sup>rd</sup> European Crystallographic Meeting, Versailles (France), August 23-27, 2022.*

- Microsymposium: Solving Structures Through Combination of Reciprocal and Direct Space Methods'

*17<sup>th</sup> European Powder Diffraction Conference (EPDIC17), Sibenik (Croatia), May 31- June 03, 2022.*

- Microsymposium: 'Progress in structure solution and refinement'

*25<sup>th</sup> Congress of the International Union of Crystallography, IUCr 2021, Prague (Czech Republic), August 14-22, 2021*

- Microsymposium: 'Structure solution and poorly crystalline materials'

*Scientific Chair of the Italian Crystallographic Association (AIC) International Crystallography School 2018, Bari (Italy), August 29–September 2, 2018*

*16<sup>th</sup> European Powder Diffraction Conference (EPDIC16), Edinburgh (UK), July 1-4, 2018*

- Microsymposium: 'Methods in structure solution and refinement'

*15<sup>th</sup> European Powder Diffraction Conference (EPDIC15), Bari, Italy, 12-15 June 2016*

- More than 350 researchers, involved in powder diffraction, participated in the EPDIC15 Congress, which had a great success, scientific as well as organizational.

*XLIV Congress of the Italian Crystallographic Association (AIC), Vercelli (Italy), September 14-18, 2015*

- Microsymposium: 'Advanced Theoretical and Experimental Methods in Crystallography'

*European Materials Research Society 2014 Fall Meeting, Symposium 'Crystallography in materials science: novel methods for novel materials', Warsaw (Poland), September 15-19, 2014*

- Microsymposium: 'Crystallography: Its past, present and future'

*41<sup>st</sup> Congress of the Italian Crystallographic Association (AIC), Verona (Italy), September 11-14, 2012*

- Microsymposium: 'Innovative methodological developments for Crystallography'

*26<sup>th</sup> European Crystallographic Meeting, Darmstadt (Germany), August 29-September 2, 2010*

- Microsymposium: 'Recent developments in software for chemical crystallography'.

*2<sup>nd</sup> Meeting of the Italian and Spanish Crystallographic Associations (MISCA), Oviedo (Spain), June 30-July 3, 2010*

- Microsymposium: ‘Software Fayre’.

*1<sup>st</sup> Meeting of the Italian and Spanish Crystallographic Associations (MISCA), Copanello di Staletti (Italy), September 24-28, 2007*

- Microsymposium: ‘Theory and Methods in Crystallography’.

*XX Congress of the International Union of Crystallography (IUCr), Florence (Italy), August 23-31, 2005*

- Microsymposium: ‘Structure Determination from Powder Diffraction Data (inorganic)’.

## **Teaching Experience**

*Teacher, ECS7-European Crystallographic School, Lisbon (Portugal), July 10-15, 2021*

- Lecture: ‘Structure solution from powder diffraction: an overview. The software EXPO.’

*Tutor within the secondary school project ‘ALTERNANZA SCUOLA-LAVORO: UNA SFIDA PER I LICEI’ of MIUR, between Liceo scientifico “Albert Einstein” – Liceo classico “Leonardo da Vinci” in Molfetta (Bari, Italy) and IC-CNR of Bari, 2017 – present*

*Co-tutor for doctoral student (XXXIII cycle), IC-CNR, Bari (Italy), November 2017- April 2021*

- In collaboration with the Department of Pharmacy-Drug Sciences, University of Bari (Italy).

*Teacher and Tutor, ECS3-European Crystallography School, Bol, Island of Brač, Croatia, September 25 - October 2, 2016*

- Lecture: ‘Full powder pattern decomposition’
- Lecture: ‘Structure model optimization’

*Co-tutor for doctoral student (XXX cycle), IC-CNR, Bari (Italy), November 2014- 2017*

- In collaboration with the Department of Pharmacy-Drug Sciences, University of Bari (Italy).

*Tutor and supervisor for the degree thesis, IC-CNR, Bari (Italy), October 2012- 2013*

- Degree in Chemistry, Faculty of Mathematical, Physical and Natural Sciences, University of Bari (Italy).

*Teacher, ‘Synthesis and Characterization of Novel Nano-Sized Inorganic Materials’, international school organized by ‘Inorganic Chemistry Division’ of Italian Chemical Society, Bari (Italy), June 17-22, 2012*

- Lecture: ‘Introduction to XRD. The single crystal technique’
- Lecture: ‘Theoretical basis and application of powder XRD techniques’.

*Teacher & Tutor, ‘The Power of Powder Diffraction’ – 44<sup>th</sup> Course, international school organized by Ettore Majorana Centre, Erice (Italy), June 2-12, 2011*

- Lecture: ‘Crystal Structure Solution by Powder Diffraction Data in Direct and Reciprocal Space by EXPO2011’.

*Teacher, CIRCC Consorzio Interuniversitario Reattività Chimica e Catalisi (Interuniversity Consortium for Chemical Reactivity and Catalysis), Bari (Italy), November 13, 2009*

- Strategic Project “ACTIBIOMAR” of the region of Apulia.

*Teacher, International Summer School on Structure Determination from Powder Diffraction Data organized by Paul Scherrer Institute (PSI) Villigen (Switzerland), June 18-22, 2008*

- Lecture: ‘Structure solution by powder diffraction data with EXPO2008: Indexing, Intensities Extraction and Space Group Determination’.

*Teacher, CIRCC Consorzio Interuniversitario Reattività Chimica e Catalisi (Interuniversity Consortium for Chemical Reactivity and Catalysis), Bari (Italy), February 25-26, 2008*

- Strategic Project “ACTIBIOMAR” of the region of Apulia.

*Teacher, Institute of Crystallography-CNR, training class within the MIUR (Ministry of Education, University and Research) Research Project, May 17-June 17, 2006.*

- Project: ‘TECSIS: Tecnologie Diagnostiche e sistemi intelligenti per lo sviluppo di parchi archeologici del Sud d'Italia (TECSIS: Diagnostic technologies and intelligent systems for the development of archaeological parks of Southern Italy)’.

*Teacher, V Experimental School on Energy Dispersion (EDXD) and Angle Dispersion (ADXD) X-ray Diffraction, Rome (Italy), September 8-20, 2003*

*Teacher, ‘Diffraction by polycrystal materials: Recent Developments of the Resolution Techniques and Structure Refinement’ school organized by Italian Crystallographic Association (AIC), Perugia (Italy), September 8-12, 1998*

*Tutor, IRMEC-CNR, March 1995 – February 1996*

- Tutored Dr. James Foadi and Dr. Anna Grazia Moliterni.

*Tutor, Crystallography Experimental School organized by the Institute of Structural Chemistry of CNR, Monterotondo, Rome (Italy), November 6-10, 1995*

*Teacher in experimental sessions (by using the instrumentation of the IC-CNR) for students of the degree courses held by Prof. C. Giacobazzo, Full Ordinary Professor of Mineralogy at the University of Bari (Italy), 1994-2011*

## **Acknowledgements**

*‘Phasing in Crystallography A Modern Perspective’, C. Giacobazzo, Oxford University Press, Oxford, 2014, ISBN 978-10-19-968699-5*

- Received thanks from Prof. C. Giacobazzo in this book.

*‘Direct Phasing in Crystallography: Fundamentals and Applications’, C. Giacobazzo, Oxford University Press, Oxford, 1998, ISBN-10: 0198500726*

- Received acknowledgements and thanks from Prof. C. Giacobazzo in this book.

*‘Direct Methods and Powder Data: State of Art and Perspectives’, C. Giacobazzo, Acta Cryst. (1996). A52, 331-339*

- Received thanks from Prof. C. Giacobazzo in this Topical Review.

## **Awards & Honors**

*Recipient of Mario Mammi AIC (Italian Crystallographic Association) Award, Fifth Meeting of the Italian and Spanish Crystallographic Associations (MISCA V), Naples (Italy), September 2019.*

*As Chair of the 15th European Powder Diffraction Conference (EPDIC15), held in Bari, Italy, 12-15 June 2016, she received Thanks and Solemn Commendation from the Director of the Institute of Crystallography of CNR of Italy, Dr. Michele Saviano, and the Chair of the European Powder Diffraction Conference Committee, Prof. Paolo Scardi for the success, scientific and organizational of the Conference.*

*Recipient of the AIC (Italian Crystallographic Association) Prize for ‘The Activity and The Original and Innovative Research Results in the Field of Crystallographic Methodologies, both Theoretical and Applicative and for the Work on the Association Activities’, XXIX National Congress of Crystallography, Naples (Italy), September 1999.*



## **Participation in Commission/Committee activities**

*Member of the jury assigning best poster prizes, sponsored by STOE, ICDD and Bruker at the 17<sup>th</sup> European Powder Diffraction Conference (EPDIC17), Sibenik (Croatia), May 31- June 03, 2022.*

*Member of the Executive Committee of the International Union of Crystallography (IUCr), 2021-*

*President of the Italian Crystallographic Association (AIC), 2021-*

*Referee for the evaluation of research products (VQR 2015-2019) on behalf of ANVUR (National Agency of the Research and University System Evaluation)*

*Member of the Commission for the participation of National Research Council of Italy to the International Union of Crystallography, April 2019 -*

*Guest Editor of Crystals, Special Issue on 'Crystal Structure Characterization by Powder Diffraction', January-December 2019*

*Main editor of Acta Crystallographica Section A, December 2018 – present*

*External reviewer of Dr. Martina Vrankić's research for the promotion to Research Associate in the Division of Materials Physics at the Ruđer Bošković Institute in Zagreb, Croatia, (request from Dr. Jasminka Popović, senior scientific associate, Head of Laboratory for synthesis and crystallography of functional materials Division for Materials Physics, Ruđer Bošković Institute, Zagreb, Croatia) 11 May 2018*

*Member of the Council of the Italian Crystallographic Association (AIC), 2018 – present*

*External reviewer of Dr. Jasminka Popović's research for the promotion to Senior Research Associate in the Division of Materials Physics at the Ruđer Bošković Institute in Zagreb, Croatia (request from Prof. Goran Štefanić, Chair of the Committee for the employment of a Senior Research Associate in the Division of Materials Physics at the Ruđer Bošković Institute in Zagreb, Croatia), 2 November 2016*

*Editor of Powder Diffraction Journal for the publication of the Proceedings of the 15th European Powder Diffraction Conference (EPDIC15), 2016 – 2017*

*External reviewer of Dr. Jimmy Xu's research for the promotion to Full Professor at Buffalo State College (request from Prof. Jane R. Cushman, Associate Professor, Chair of the Mathematics Department, Buffalo State College), 19 September 2016*

*Referee for the evaluation of research products (VQR 2011-2014) on behalf of ANVUR (National Agency of the Research and University System Evaluation)*

*Co-editor of Acta Crystallographica Section A, 2014 – present*

*Member of the European Powder Diffraction Conference (EPDIC) Committee, 2016 - present*

*Member of the Commission on Powder Diffraction (CPD) of the International Union of Crystallography (IUCr), 2014 – present*

*Referee of the following international peer reviewed Journals:*

- Acta Crystallographica Section A
- Journal of Applied Crystallography
- Crystals
- Zeitschrift für Kristallographie
- EPDIC Proceedings
- Journal of Physical Chemistry
- Macromolecules

- Journal of Alloys and Compounds
- Journal of Solid State Chemistry
- Polyhedron
- Powder Diffraction
- Thermochimica Acta
- Macedonian Journal of Chemistry and Chemical Engineering
- Crystal Growth and Design
- Crystal Research and Technology
- Nuclear Inst. and Methods in Physics Research
- Journal of Nanomaterials
- Inorganic Chemistry

*Member, Organizing, Scientific or Steering Committee for the following:*

- European Materials Research Society 2021 Fall Meeting Symposium H ‘Modern computational methods and their applications in materials science: Synergy of theory and experiment’, On-line, September 20-23, 2021
- XLIX AIC (Italian Crystallographic Association) National Congress, Parma (Italy), September 6-8, 2021
- AIC International Crystallography School 2018, Bari (Italy), August 29–September 2, 2018
- 3rd Joint AIC-SILS Conference, Rome (Italy), June 25-28, 2018
- ECS3-European Crystallography School, Bol, Island of Brač, Croatia, September 25 - October 2, 2016
- 15<sup>th</sup> European Powder Diffraction Conference (EPDIC15), Bari, Italy, June 12-15, 2016
- XLIV AIC National Congress, Vercelli (Italy), September 14-18, 2015
- International EXPO/SIR Workshop organized by IC-CNR, Bari (Italy), June 10-13, 2014
- 41<sup>st</sup> Congress of the Italian Crystallographic Association (AIC), Verona (Italy), September 11-14, 2012
- International workshop ‘PHARE 2009 A modular workshop on global PHase REtrieval (Modulo 1-Crystal structure solution and refinement from powder data)’ organized by IC-CNR, Martina Franca (Italy), April 15-17, 2009
- 1<sup>st</sup> Meeting of the Italian & Spanish Crystallographic Associations, Copanello di Staletti (Italy), September 24-28, 2007
- XXX AIC (Italian Crystallographic Association) National Congress, Martina Franca (Italy), September 19-22, 2000
- V SIR Workshop ‘SIRWARE96: Single Crystal and Powder Data X-Rays, neutrons and electrons’, international workshop organized by IRMEC-CNR, Bari (Italy), December 17-20, 1996
- IV SIR Workshop: ‘SIR92-SIRPOW.92: two powerful tools for solving crystal structure via single crystal and powder data’, international workshop organized by IRMEC-CNR, Bari (Italy), April 5-7, 1993

*Member of the President Council of the Italian Crystallographic Association (AIC), 2003-2005*

*Member of the European Crystallographic Association (ECA), 1997-2016*

*Member, Scientific Council of the Institute for the Development of Crystallographic Methodologies of the National Research Council of Italy (IRMEC-CNR), Bari (Italy), February 1994- February 2001*

*Member, Italian Crystallographic Association (AIC), 1989-present*

*Member, Examining Commission for the following:*

- Assigning a CNR Research Grant, FIRB-MIUR research project, at IC-CNR according to the selection notice n. 004/2013 BA, prot. N. 0001453 (October 21, 2013), November 2013
- Assigning a CNR Research Grant, PON01\_00625 research project, at IC-CNR according to the selection notice n. 006/2012 BA prot. N. 0001087 (July 6, 2012), September 2012
- Assigning ‘Nardelli Prize’ of the Italian Crystallographic Association (AIC), June 2012

- Assigning a CNR Research Grant, FIRB-MIUR research project, at IC-CNR according to the selection notice n. 01/2010 prot. N. 0001451 (October 6, 2010), November 16, 2010
- Assigning a CNR Research Grant to computer scientist at IC-CNR according to the selection notice n. 6/2009 prot. 0000791 (September 30, 2009), October 22, 2009
- Assigning permanent position as Research Scientist at IC-CNR according to the selection notice prot. n. 752 (November 27, 2007), December 13, 2007
- Assigning a Research Grant at IC-CNR according to Project 'Marie Curie host fellowships' in 'Improving the Human Research Potential and the Socio-Economic Knowledge Base' (027/CO/08, 027/CO/09, November 11, 2005), January 10, 2006
- Assigning permanent position as Research Scientist at IC-CNR according to the selection notice prot. n. 183\01\C (December 13, 2001), December 18-19, 2001.
- Assigning permanent position as technician at IC-CNR according to the selection notice prot. n. 82\01\C (September 13, 2001), October 8, 2001.

*Coordinator of the topic on 'Crystallographic Methodologies' for the section 'Crystallography in Italy' in the 'International Union of Crystallography (IUCr) Newsletter', 2004.*

## **RESEARCH ACTIVITY**

Dr. Altomare has a high scientific competence in the development of crystallographic methodologies aimed at structural characterization of crystalline compounds (single crystal and microcrystalline powders). This expertise is widely recognized by the scientific community at national and international levels, as proved by the large number of citations that her publications have received. Dr. Altomare is leader of a research team of the Institute of Crystallography of the Italian National Council of Research, mainly devoted to powder diffraction analyses. The research of Dr. Altomare is of both theoretical and applicative interest. In particular, it covers a broad spectrum of applications (organic, inorganic, innovative and technologically interesting compounds, minerals, drugs ...). Dr. Altomare has also gained experience in the planning and governance of research projects.

Dr. Altomare is co-author of twelve important crystallographic computing programs widely used by national and international scientific community: *SIR92*, *SIRPOW92*, *EXTRA*, *SIR97*, *EXPO*, *QUANTO*, *EXPO2004*, *QUALX*, *EXPO2009*, *EXPO2013*, *QUALX2.0*, *OChemDb*. The programs are illustrated in scientific paper publications in JCR Journals. The scientific publications illustrating each developed software package are listed below.

### **1. *OChemDB***

Scientific paper: **A. Altomare, N. Corriero, C. Cuocci, A. Falcicchio, A. Moliterni & R. Rizzi** (2018)

OChemDb: the free online Open Chemistry Database portal for searching and analysing crystal structure information

**J. Appl. Cryst.**, 51, 1229-1236.

### **2. *QUALX2.0* (updated version of *QUALX*).**

Scientific paper: **A. Altomare, N. Corriero, C. Cuocci, A. Falcicchio, A. Moliterni & R. Rizzi** (2015)

*QUALX2.0*: a qualitative phase analysis software using the freely available database POW\_COD

**J. Appl. Cryst.**, 48, 598-603.

### **3. *EXPO2013* (updated version of *EXPO2009*, improved by graphical and computational performances and supported by new methodological approaches).**

Scientific paper: **A. Altomare, C. Cuocci, C. Giacobozzo, A. Moliterni, R. Rizzi, N. Corriero & A. Falcicchio** (2013)

*EXPO2013*: a kit of tools for phasing crystal structures from powder data

**J. Appl. Cryst.** 46, 1231-1235.

*EXPO2013* has been integrated in software provided by japanese RIGAKU Corporation.

4. **EXPO2009** (software for structure solution by powder diffraction data, able to indexing, determining the space group, extracting the integrated intensities, solving the structure by Direct Methods and/or Direct Space Methods, refining the structure model by Rietveld method).  
Scientific paper: A. Altomare, C. Cuocci, C. Giacovazzo, A. Moliterni & R. Rizzi (2009)  
*EXPO2009*: structure solution by powder data in direct and reciprocal space  
*J. Appl. Cryst.* 42, 1197-1202.  
**EXPO2009 has been integrated in software provided by Japanese RIGAKU Corporation.**
5. **QUALX** (software for qualitative analysis of powder compounds).  
Scientific paper: A. Altomare, C. Cuocci, C. Giacovazzo, A. Moliterni & R. Rizzi (2008)  
*QUALX*: a computer program for qualitative analysis using powder diffraction data  
*J. Appl. Cryst.* 41, 815-817.
6. **EXPO2004** (software for structure solution by powder diffraction data, able to indexing, determining the space group, extracting the integrated intensities, solving the structure by Direct Methods, refining the structure model by Rietveld method).  
Scientific paper: A. Altomare, R. Caliendo, M. Camalli, C. Cuocci, C. Giacovazzo, A.G.G. Moliterni & R. Rizzi (2004)  
Automatic structure determination from powder data with *EXPO2004*  
*J. Appl. Cryst.* 37, 1025-1028.
7. **Quanto** (software for quantitative analysis of powder multiphase mixture).  
Scientific paper: A. Altomare, M.C. Burla, C. Giacovazzo, A. Guagliardi, A.G.G. Moliterni, G. Polidori & R. Rizzi (2001)  
*Quanto*: A Rietveld Program for quantitative phase analysis of polycrystalline mixture  
*J. Appl. Cryst.* 34, 392-397.
8. **EXPO** (software for extracting the integrated intensities from powder diffraction pattern and solving structure by Direct Methods).  
Scientific paper: A. Altomare, M. C. Burla, M. Camalli, B. Carrozzini, G. L. Cascarano, C. Giacovazzo, A. Guagliardi, A. G. G. Moliterni, G. Polidori & R. Rizzi (1999)  
*EXPO*: a program for full powder pattern decomposition and crystal structure solution  
*J. Appl. Cryst.* 32, 339-340.
9. **SIR97** (Direct Methods software for structure solution by single crystal data).  
Scientific paper: A. Altomare, M. C. Burla, M. Camalli, G. L. Cascarano, C. Giacovazzo, A. Guagliardi, A. G. G. Moliterni, G. Polidori & R. Spagna (1999)  
*SIR97*: a new tool for crystal structure determination and refinement  
*J. Appl. Cryst.* 32, 115-119.  
**SIR97 has been integrated in software provided by MSC-Rigaku, Enraf-Nonius, MAC Science companies.**
10. **EXTRA** (software for extracting the integrated intensities from powder diffraction pattern).  
Scientific paper: A. Altomare, M.C. Burla, G. Cascarano, C. Giacovazzo, A. Guagliardi, A.G.G. Moliterni & G. Polidori (1995)  
*EXTRA*: a program for extracting structure-factor amplitudes from powder diffraction data  
*J. Appl. Cryst.* 28, 842-846.
11. **SIRPOW.92** (Direct Methods software for structure solution by powder diffraction data).  
Scientific paper: A. Altomare, G. Cascarano, C. Giacovazzo, A. Guagliardi, M.C. Burla, G. Polidori, M. Camalli (1994)  
*SIRPOW.92* - A program for automatic solution of crystal structures by direct methods optimized for powder data  
*J. Appl. Cryst.* 27, 435-436.
12. **SIR92** (Direct Methods software for structure solution by single crystal data).  
Scientific paper: A. Altomare, G. Cascarano, C. Giacovazzo, A. Guagliardi, M.C. Burla, G. Polidori & M. Camalli (1994)  
*SIR92* - a program for automatic solution of crystal structures by direct methods  
*J. Appl. Cryst.* 27, 435.  
**SIR92 has been integrated in software provided by MSC-Rigaku, Enraf-Nonius, MAC Science companies.**

Dr. Altomare's research activity is presented in:

- 133 scientific publications in international JCR journals
- 10 chapters of books
- 12 computing programs used worldwide
- several communications as oral contributions, many of them on invitation, in national and international congresses and schools, several poster contributions, and participations in congresses.
- H-index: 35 (Google Scholar, September 2022).
- **Number of citations: 31969** (Google Scholar, September 2022).

