PERSONAL INFORMATION

Anna Moliterni

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https://orcid.org/0000-0001-6786-6982

Sex Female | *Date of birth* 02/07/1967 | *Nationality* Italian

Enterprise	University	EPR
☐ Management Level	☐ Full professor	☐ Research Director and 1st level Technologist / First Researcher and 2nd level Technologist
☐ Mid-Management Level	☐ Associate Professor	☒ Level III Researcher and Technologist
☐ Employee / worker level	☐ Researcher and Technologist of IV, V, VI and VII level / Technical collaborator	☐ Researcher and Technologist of IV, V, VI and VII level / Technical collaborator

WORK EXPERIENCE

February 2001 – Present

Researcher (full time/permanent position)

Institute of Crystallography (IC)- CNR
Via G. Amendola 122/O - 70126 Bari – Italy

- **Main activities**: *Ab-initio* structure solution of crystalline materials with different chemical composition and complexity *via* powder and/or single crystal diffraction data; development and implementation in crystallographic software of innovative theoretical, methodological and computing tools devoted to 1) structure solution and refinement by single crystal diffraction data; 2) structure solution and refinement by powder diffraction data; 3) qualitative phase analysis by powder data; 4) quantitative phase analysis by powder data.
  In case of powder diffraction data, her research activity covers the following topics: indexing, space group determination, structure solution by traditional methods (direct methods and Patterson methods) and global optimization methods, structural optimization and Rietveld analysis, phase identification.
  The expertise of Dr. Moliterni in the field of the structure characterization of crystalline materials by powder and single crystal diffraction data is furtherly proved by some recent publications on relevant ISI journals, emphasizing the key role of Crystallography in the structure characterization of amazing and challenging new compounds like 2D organic-inorganic hybrid perovskites [see https://www.psi.ch/en/macromolecular-crystallography/scientific-highlights/lighting-up-the-appealing-world-of-hybrid; *Adv. Mater*. (2022). **34**, 2106160] and nanocrystalline metal chalcohalides [see https://www.cnr.it/it/comunicato-stampa/11017/nanomateriali-inesplorati-per-semiconduttori-senza-piombo; *Angew. Chem. Int. Ed*. (2022). **61**, e202201747; *Nat. Comm.* (2022). **13**, 3976].

- **Since March 2004, Dr. Moliterni is faulty in charge of the X-ray single crystal diffraction laboratory** at the IC-CNR of Bari (KappaCCD Bruker-Nonius diffractometer).

- The interdisciplinary character of the research activity of Dr. Moliterni is confirmed by her participation in research projects funded in different scientific fields (*e.g.*, Materials Science, Biomedicine, Pharmaceutical Chemistry, Cultural Heritage, ..).

The research activity of Dr. Moliterni is documented by:

- **Bibliometric parameters (December, 2023):**

ISI Web of Knowledge source:
Overall number of publications: **150** documents, H-index = **29**; Sum of Times Cited (Without self citations): **> 13200**, Citing articles (Without self citations) **> 12500**;

Scopus source (Scopus Author ID: 7004663206)
Overall number of publications: **123** documents, H-index = **26**; number of citations **> 13100,** Co-authors: **> 290**.

Google Scholar source:
Overall number of publications: **195** documents, H-index = **32**; number of citations **> 25800.**

- **Seven book chapters**, two of them published in 2019 on a new volume of the *International Tables for Crystallography*, dedicated to powder diffraction (Volume H); this volume covers the powder diffraction technique with over 50 chapters written by experts in the field: https://it.iucr.org/H/;

- **Co-authorship of ten crystallographic computing programs,** here listed according to software distribution decreasing years: **OChemDb, QUALX2.0, EXPO2014, EXPO2009, QUALX, EXPO2004, Quanto, EXPO, SIR97, EXTRA**, in which innovative methods and algorithms have been implemented. These programs are widely used by the national and international scientific community, and are distributed by the website of the Institute of Crystallography (IC)- CNR, Bari, Italy (http://www.ba.ic.cnr.it/softwareic/). In particular:
  a) the numbers concerning the total citations and registered users of the computing programs belonging to the "EXPO family" (aimed at the structure solution by powder diffraction data) are greater than 1500 and 6800, respectively;
  b) the numbers concerning the total citations and registered users of the computing programs devoted to qualitative phase analysis (*i.e.*, QUALX2.0 and QUALX) are greater than 230 and 12800, respectively;
  c) in the case of the software SIR97 the number of citations is about 9500.

- **CNR award:**
On October 1, 2009, Dr. Moliterni was the winner of one of the 100 awards for CNR researchers and technologists; the award was given to her *'for having achieved, in 2005, innovative results of particular excellence and strategic importance*'.

- Since 2022**, Scientific Expert for the Evaluation of Project Proposals** (MISE – Ministry of Enterprises and Made in Italy- Fund for Sustainable Growth).

- **Patent:**
A. Moliterni is co-inventor on a provisional patent application entitled 'Process for the Production of Nanocrystals of Metal Chalcohalides', PCT/IB2023/050820.
https://www.knowledge-share.eu/brevetto/processo-per-la-produzione-di-nanocristalli-di-calcoalogenuri-metallici/

- **Numerous oral communications held at national and international congresses and workshops** (some of which were invited lectures). In particular,

Invited Lectures:

- **A. Moliterni**: 'Crystallography - a powerful lens for Materials Science', 28th Croatian-Slovenian Crystallographic Meeting (CSCM28), 7-11 September 2022, Poreč, Croatia. **(Plenary lecture)**
- **A. Moliterni**: 'Crystallography sheds light on the fascinating world of perovskites', UNIMORE, University of Modena and Reggio Emilia, 14 June 2022, Modena, Italy.
- **A. Moliterni**: 'Single Crystal X-Ray Crystallography lights up pharmaceutical compounds: main investigations and structural insights', Bridging structural biology and drug discovery - II, 2nd Joined Workshop between the Institute of Crystallography (CNR) and the Department of Pharmacy – Pharmaceutical Sciences (UNIBA), 11 May 2022, Bari, Italy.
- **A. Moliterni**, D. Altamura, R. Lassandro, V. Olieric, C. Giannini: 'Structure investigation of challenging organic and hybrid compounds by single crystal synchrotron microdiffraction', 4th Edition of the International Virtual Conference on Materials & Environmental Science, ICMES-2020 'New Materials for Sustainable Energy Development', November 18-27, 2020, Oujda, Morocco.
- **A. Moliterni**: 'EXPO: a powerful tool for solving powder crystal structures in direct and reciprocal space', International Meeting 'Crystal Forms @ Bologna', Bologna, Italy, 19-21January 2012.
- **A. Moliterni**, A. Altomare, C. Cuocci, C. Giacovazzo, R. Rizzi: 'Ab-initio structure determination by powders: recent developments in EXPO2010', 26th European Crystallographic Meeting, Darmstadt,

Germany, 29 August-02 September 2010.

- A. Altomare, C. Cuocci, C. Giacovazzo, **A. Moliterni**, R. Rizzi: 'Crystal structure determination by powder diffraction data in direct and reciprocal space by EXPO2009', 19th National Meeting of the Brasilian Crystallographic Association (ABCr), 19a Reuniao de ABCr, Belo Horizonte, Brasil, 8-11 September 2009. **(Plenary lecture)**

- **A. Moliterni**: 'EXPO: Nella cassetta degli attrezzi', Powder Diffraction Workshop 'In the toolchest', Warsaw, held during the EPDIC11 (11-th European Powder Diffraction Conference), Warsaw, 19-22 September 2008.

- **A. G. Moliterni**, A. Altomare, R. Caliandro, M. Camalli, C. Cuocci, C. Giacovazzo, R. Rizzi: 'New Strategies for the ab-initio Structure Solution in EXPO2005', XX Congress of the International Union of Crystallography, Florence, 23-31 August 2005.

- **A. Moliterni**: 'Ab-initio structure determination from powder data by EXPO: from indexing to structure solution', 16 May 2001, University of Stockholm, Department of Structural Chemistry, Stockholm, Sweden.

Lectures at International Congresses and Workshops:

- **A. Moliterni**, D. Altamura, R. Caliandro, C. Giannini ' "Disentangling the structure of nanocrystalline materials for Energy by Crystallography", 2023 FALL MEETING of the European Materials Research Society (E-MRS), September 18 -21 2023, Warsaw, Poland.

- **A. Moliterni**: 'Indexing', EXPO and more International Workshop, 30 September - 3 October 2019, Bari, Italy. (Lecturer and tutor).

- **A. Moliterni**: 'Space group determination', EXPO and more International Workshop, 30 September 3 October 2019, Bari, Italy. (Lecturer and tutor).

- **A. Moliterni**: 'QUALX2.0: a qualitative phase analysis software', Software Fayre held during the International Conference EPDIC16, 1-4 July 2018, Edinburgh, United Kingdom.

- **A. Moliterni**: 'QualX2: qualitative phase analysis', Crystallographic Software Fayre, held during the International Conference 29th European Crystallographic Meeting (ECM29), August 23-28, 2015, Rovinj, Croatia.

- **A. G. Moliterni**: 'Characterization of crystalline materials of interest for Cultural Heritage by X-Ray powder diffraction', International Conference 'Preservation and Enhancement in Cultural Heritage - The 'T.He.T.A.' project and research experiences in the European context', Gioia del Colle, October 21-22, 2014.

- **A. Moliterni**: 'Unit Cell Identification', International EXPO/SIR Workshop – Module 1, 10-11 June 2014, Bari, Italy. (Lecturer and tutor).

- **A. Moliterni**: 'Rietveld refinement', International EXPO/SIR Workshop – Module 1, 10-11 June 2014, Bari, Italy. (Lecturer and tutor).

- **A. Moliterni**: 'The random-model-based method (RAMM) in EXPO2013', 'The Twentysecond Croatian-Slovenian Crystallographyc Meeting (CSCM22)', Biograd, Croatia, June 12-16, 2013.

- **A. Moliterni**: 'EXPO, structure solution in direct and reciprocal space', EPDIC13 Lachlan's Software Fayre, EPDIC13, Grenoble, 28-31 October 2012.

- **A. Moliterni**: 'EXPO2011', Cystallographic Software Fayre, XXII Congress and General Assembly of the International Union of Crystallography, Madrid, Spain, 22-30 August 2011.

- **A. Moliterni**, A. Altomare, G. Campi, C. Cuocci, L. Eriksson, C. Giacovazzo, R. Rizzi: 'New Frontiers in Powder Diffraction Pattern Indexing: the Program N-TREOR09', 25th European Crystallographic Meeting, Istanbul, Turkey, 16-21 August 2009.

- **A. Moliterni**: 'EXPO2009 for powder diffraction data', Cystallographic Software Fayre, Istanbul, Turkey, 18th-19th August 2009, held during the '25th European Crystallographic Meeting' (ECM25), Istanbul, 16 - 21 August 2009.

- **A. Moliterni**: 'The recipes for a friendly use of EXPO2009', International Workshop 'PHARE2009, A modular workshop on PHAse Retrieval, Module 1- Crystal structure solution and refinement from powder data', 15-17 April 2009, Martina Franca, Italy. (Lecturer and tutor).

- **A. Moliterni**: 'Indexing by NTREOR09', International Workshop 'PHARE 2009, A modular workshop on PHAse Retrieval, Module 1- Crystal structure solution and refinement from powder data', 15-17 April 2009, Martina Franca, Italy. (Lecturer and tutor).

- **A. G. Moliterni**: 'Preferred Orientation', International Workshop 'The Fifth SIR Workshop - SIRWARE 96', Bari - Italy, 17-20 December 1996. (Lecturer and tutor).

- **A. G. Moliterni**: 'Special features of SIRPOW.97', International Workshop 'The Fifth SIR Workshop SIRWARE 96', Bari - Italy, 17-20 December 1996. (Lecturer and tutor).

Lectures at National Congresses:

- **A. Moliterni**, C. Giannini: 'Unveiling the crystal structure of novel hybrid organic-inorganic perovskites by synchrotron X-ray powder/single crystal diffraction data', SILS Conference 2023, August 30th – September 1st, Roma.

- **A. Moliterni**: 'Exploring the amazing world of perovskites by the powerful lens of Crystallography', Conferenza di Dipartimento DSCTM, 13-15 Dicembre 2021, Aula Marconi - CNR, Roma.

- **A. Moliterni**, S. Toso, E. Mugnaioli, J. Ramade, S. Bals, M. Gemmi, L. Manna, C. Giannini: '3D electron and X-ray powder diffraction multi-technique approach for structural investigation of new challenging lead chalcohalide nanocrystals', First Conference on Crystallography, Structural Chemistry and Biosystems, Catania, October 4-6, 2021.

- **A. Moliterni**, S. Toso, E. Mugnaioli, J. Ramade, S. Bals, M. Gemmi, L. Manna, C. Giannini: 'Structural investigation of new challenging lead chalcohalide nanocrystals by combining 3D electron and X-ray powder diffraction', SILS Meeting 2021, Bologna, June 21-23.

- **A. Moliterni**, D. Altamura, V. Olieric, A. Camposeo, D. Pisignano, D.B. Granger, S.R. Parkin, J.E. Anthony, C. Giannini: 'Single-crystal synchrotron X-ray diffraction study of new anthracene derivatives compounds', SILS 2019 Meeting, Camerino, 9-11 September 2019.

- A. Altomare, C. Giacovazzo, M. Ianigro, **A.G.G. Moliterni**, R. Rizzi: 'The use of crystal chemical information in EXPO2001: a new peak labelling algorithm', XXXI Congresso Nazionale dell'Associazione Italiana di Cristallografia, Parma, 18-21/9/2001.

- A. Altomare, C. Giacovazzo, A. Guagliardi, **A.G.G. Moliterni**, R. Rizzi: 'Nuove frontiere di EXPO: dall' indicizzazione di un pattern di diffrazione alla soluzione strutturale', XXIX Congresso Nazionale dell'Associazione Italiana di Cristallografia, Napoli, 7-9/09/1999.

- A. Altomare, M. C. Burla, M. Camalli, B. Carrozzini, G. Cascarano, C. Giacovazzo, A. Guagliardi, **A.G.G. Moliterni**, G. Polidori, R. Rizzi: 'Nuovi sviluppi nella soluzione ab initio di strutture cristalline da dati da polveri: il package EXPO', XXVII Congresso Nazionale dell'Associazione Italiana di Cristallografia, Perugia, 12-14/09/1997.

- A. Altomare, G. Cascarano, C. Giacovazzo, A. Guagliardi, **A.G.G. Moliterni**, M. C. Burla, G. Polidori: 'Finding the number of statistically independent observations in a powders diffraction pattern. The algorithm and the first applications', XXV Congresso Nazionale dell'Associazione Italiana di Cristallografia, Giardini-Naxos, 25-27/09/1995.

- **Organization of national and international congresses, and international crystallography workshops:**

- **Member of the Scientific Committee** of the 5th International Conference on Materials & Environmental Science (ICMES 2022), June 09-12, 2022, Saïdia, Morocco (Conference (mocedes.org)).

- **Organizer** of the Joined Workshop between the Institute of Crystallography–CNR and the Institute of Materials Science, Technische Universitat (TU) Dresden, 1st July 2022 (https://eventi.mlib.ic.cnr.it/event/39).

- **Member of the International Scientific Committee** of the 4th International Virtual Conference on Materials & Environmental Science (ICMES 2020), 18-28 November 2020 (Conference (mocedes.org)).

- **Member of the Local Organizing Committee** of the European Powder Diffraction Conference – EPDIC15, Bari, Italy, 12-15 June 2016.

- **Member of the Organizing and Scientific Committee** of the Workshop: 'International EXPO/SIR Workshop – Module 1', 10-11 June 2014, Bari - Italy.

- **Organizer** of the International Workshop 'PHARE 2009 A modular workshop on global PHAse REtrieval' -(Module 1 – Crystal structure solution and refinement from powder data), 15-17 April 2009, Martina Franca (TA), Italy.

- **Member of the Program Committee** of the XXXV Congress of the Italian Crystallographic Association (AIC), Ferrara, 18-21 September, 2006.

- **Member of the Organizing Committee** of the XXX Congress of the Italian Crystallographic Association (AIC), Martina Franca (TA), Italy, 19-22 September 2000.

- **Organizer** of the Fifth SIR Workshop 'SIRWARE96: Single Crystal and Powder Data X-Rays, Neutrons and Electrons', Bari, Italy, 17-20 December 1996.

- **Organizer** of the Fourth SIR Workshop 'SIR92-SIRPOW.92, two powerful tools for solving crystal structures via single crystal and powder data', Bari, Italy, 5-7 April 1993.

- Chairing Sessions:

- **Chairman** of Session 2 of the Joined Workshop between the Institute of Crystallography–CNR and the Institute of Materials Science, Technische Universitat (TU) Dresden**,** 1st July 2022 (https://eventi.mlib.ic.cnr.it/event/39).

- **Chairman** of the Session H. 'Software/Tools to Deal with Crystal and Crystallographic Issues & Teaching Crystallography', The 2nd International Online Conference on Crystals, 10-20 November 2020, sciforum, Crystals 2020.

- **Chairman of the Microsymposium MS6** 'Frontier Methods in structural determination', MISCA2016 Congress, IV Meeting of the Italian and Spanish Crystallographic Associations, 21st-25th June 2016, Tenerife, Spain.

- **Chairman of the Microsymposium MS2** 'Ab initio Structure Solution', European Powder Diffraction Conference - EPDIC13, Grenoble, 28-31 October 2012.

- **Chairman of the Microsymposium MS6** 'Recent Developments in Powder Crystallography', XXXV Congress of the Italian Crystallographic Association (AIC), Ferrara, 18-21 September 2006.

- Organization of International Schools, Chairing Teaching Activities and Commissions:

- **Chair of the Local Organizing Committee** of the AIC International Crystallography School 2018 (AICS2018) 'Powder Diffraction: Theory, Software and Applications', 29 August-02 September 2018, Bari, Italy.

- **Chair of the Teaching Committee of the Italian Crystallographic Association** (January 2015 - December 2017).

- **Organizer** of the AIC International School 2017 'Bridging the gap between cryo-EM and crystallography', Pavia, 3-6 September 2017.

- **Member of the Scientific and Organizing Committee** of the AIC International Crystallography School 2016 'Polymorphism, Stability and Phase Transitions in Crystals – theory, experiments, applications', 7-11 September 2016, Rimini, Italy.

- **Member of the Organizing Committee** of the 1st European School on Crystal Growth (ESCG), 5-8 September 2015, Bologna.

- **Member of Teaching Commission of the Italian Crystallographic Association (AIC)** (January 2012 - December 2014).

- **Member of the Scientific and Organizing Committee** of the 1st European Crystallographic School (ECS1) 'Reinforcing foundations to build the 2nd century of modern crystallography', Pavia, 28 August - 6 September 2014.

- **Member of the Organizing Committee** of the 1st joint SIMP-AIC International School 'Crystallography Beyond Diffraction 2nd edition', Camerino, 4-8 September 2013.

- **Member of the Scientific and Organizing Committee** of the AIC International School - 10th edition 'Paolo Giordano Orsini' School titled 'Structure, Microstructure, Nanostructure – exploiting the potential of powder diffraction techniques', Trento, 15-20 September 2012.

-Teaching activities (also by invitation) **in national, international schools and crystallography courses:**

- **A. Moliterni**: 'Combining synchrotron radiation and Crystallography to decrypt the structure of materials impacting Energy, Environment and Health', XVI School on Synchrotron Radiation: Fundamentals, Methods and Applications, Trieste, Italy, 19-30 September 2022. (**Invited Lecture**)

- **A. Moliterni**: 'Indexing and space group determination', ECS3 – 3rd European Crystallography School, September 25 – October 2, 2016, Bol, Island of Brač, Croatia. (**Invited Lecture**)

- **A. Moliterni**: **Course** titled 'Ab-initio structure determination by powder diffraction data', held during the 19th National Meeting of the Brazilian Crystallographic Association (19a Reunião de ABCr), Belo Horizonte, Brazil, 8-11 September 2009. (**Invited Course**)

- **A. Moliterni**: 'Qualitative phase analysis by XRPD', 1st joint SIMP-AIC International School 'Crystallography Beyond Diffraction 2nd edition', Camerino, 4-8 September 2013.

- **A. Moliterni**: **Course** consisting of three Lectures [1) Tecniche diffrattometriche da cristallo singolo I; 2) Tecniche diffrattometriche da polveri cristalline I; 3) utilizzo del software EXPO2009]; the Course has been required by CIRCC (Consorzio Interuniversitario Reattività Chimica e Catalisi), 23-25 November 2009, Bari. (**Invited Course**)

- **A. Moliterni**: **Course** consisting of four Lectures [1) Dal profilo di diffrazione X da polveri cristalline alla soluzione strutturale. Introduzione; 2) Dal profilo di diffrazione X da polveri cristalline alla soluzione strutturale; 3) Il programma EXPO per la soluzione strutturale. I; 4) Il programma EXPO per la soluzione strutturale. II]; the Course has been required by CIRCC (Consorzio Interuniversitario Reattività Chimica e Catalisi), 25-29 Febbraio 2008, Bari. (**Invited Course**)

- **Lecturer** at the 'Scuola tuniso-italiana d'autunno di diffrazione su polveri: risoluzione strutturale ab-initio', organized by the Tunisian Crystallographic Association, University of Monastir, Tunisia, 5-7 November 2006.

- **Lecturer** at the School organized by the Italian Crystallographic Association (AIC): 'Diffrattometria da materiali policristallini: recenti sviluppi delle tecniche di risoluzione e di raffinamento strutturale', Perugia, 8-12 September 1998 (**Invited Lesson**).

- **Tutor and responsible of the research activity** (carried out in the period 01/10/2012-31/05/2016) of **Dr. Nicola Corriero,** research fellow at the Institute of Crystallography (IC) -CNR, Bari, Italy;

- Editorial Roles for ISI journals:

- **Associate Editor** of Frontiers in Chemistry (specialty section: 'Solid State Chemistry'), IF(2021)=5.545, ISSN = 2296-2646.

- **Member of the Editorial Board** of the MDPI journal Crystals [IF(2021)=2.67, ISSN=2073-4352].

- **Member of Editors of the Special Issue of Crystals** [IF(2021)=2.67, ISSN=2073-4352]: "Selected Papers from the 2nd International Online Conference on Crystals".

- Referee for ISI journals:

1. Nanoscale; **2.** Journal of Materials Chemistry C; **3.** Scientific Reports; **4.** Journal of Applied Crystallography; **5.** Journal of Physics and Chemistry of Solids; **6.** Journal of the American Ceramic Society; **7.** Journal of Molecular Structure; **8.** Minerals; **9.** Acta Crystallographica Section B; **10.** Crystals; **11.** Acta Crystallographica Section A; **12.** Inorganica Chimica Acta; **13.** Powder Diffraction; **14.** Zeitschrift für Kristallographie; **15.** Proceedings of EPDIC-13; *16.* Periodico di Mineralogia.

- **External referee** (carried out in January 2021) for the PhD Thesis of Dr. Giancarlo Gallo, University of Salerno, Department of Chemistry and Biology 'A. Zambelli', XXXIII Doctoral Cycle in Chemistry.
Title of the PhD Thesis: 'Elucidation of Crystal Structures and Structural Changes using X-ray Powder Diffraction'.
Supervisors: Prof. Consiglia Tedesco; Prof. Robert E. Dinnebier; Dr. Bernd Hinrichsen.

- Recent Research Projects:

- **Project Prin 2022 - ERC Sector PE5 "Synthetic Chemistry and Materials -** titled 'Conjugated organic-inorganic two-dimensional halide perovskite for stable solar cells and modules (CONPER)'- Project code: **2022CBBEHN**
Dr. A. Moliterni is the person in charge of the project for the CNR unit (IC and ICCOM institutes).
Period: 18/10/2023 – 18/10/2025
Duration: 24 months

- **Bando Ricerca di Sistema - CSEA - TIPO A 2021 - Project CANVAS** titled 'nuovi Concetti, mAteriali

e tecnologie per l'iNtegrazione del fotoVoltAico negli edifici in uno scenario di generazione diffuSa' - Code CSEAA_00009; Photovoltaic Sector.
Dr. D. Altamura and Dr. A. Moliterni are persons in charge of the project for the IC-CNR unit of Bari.
Approval date: 05/08/2022; Starting date: 01/03/2023
Duration: 36 months

- **Project PNNR (Centro Nazionale 01 – CN0000013)** *National Centre for HPC, Big Data and Quantum Computing – HPC*
Dr. C. Cuocci and Dr. A. Moliterni are persons in charge of the project for the IC-CNR unit of Bari.
Period: 01/09/2022 – 31/08/2025

- **Programma "AMICO" 2-,** Programma di Applicazione, MIglioramento e COstruzione dei trovati brevettati – AMICO 2a ed., **Bando POC PNRR 2022, Progetto MEX-UP** – 'Produzione in scala di nanocristalli di calcoalogenuri metallici' (v. https://www.cnr.it/it/news/12037 e https://www.cnr.it/it/bando-uvr-amico-poc-2022)
Duration: 12 months, Approval date: 21/06/2023

- **Bilateral Project CNR-CINVESTAV (Mexico)-2023-2024** titled 'Biomineralization of eggshells of dinosaurs of 70 million years old from the northern part of Mexico'
Period: 01/01/2023 – 31/12/2024

- **Piano Operativo di Ricerca (POR) - Accordo di Programma MiTE -ENEA PNRR Investimento 3 5 -Ricerca e Sviluppo sull'Idrogeno** titled 'Research and development of technologies for the hyd rogen supply chain'
Period: 01/07/2022 – 31/12/2025

- **Project DATIAMO (call @CNR)** titled 'Development of A Technological platform for the Identification of s1R Allosteric Modulators with potent SARS-CoV-2 antiviral activity'
Period: February 2022-February 2024

- **Bilateral Project CNR/FAPESP (Brazil)-** 2022-2023 titled 'Advanced X-ray Characterization of Pb-free perovskite nanomaterials'
Period: 2022-2023

- **PON 2020-2023 –' ECOTEC'** titled 'Fibre e tessuti intelligenti ed ECOsostenibili per l'abbigliamento TECnico e l'alta moda'
Period: 18/12/2020-18/06/2023

- **Bilateral Project CNR/CNRST (Moroc)- 2020-2021** titled 'New MOFs based on Pyrazole ligand: Crystal structure and Biological evaluation (NMPCB)'
Dr. Moliterni has been the Project Leader of the IC-CNR unit.
Period: 2020-2021 (extended to 31 July 2022)

- **PON 2014-2020 - 'IDF SHARID'** titled 'Innovative Devices For SHAping the Risk of Diabetes'
Period: 04/09/2019-03/03/2022 (extended to 03/09/2022)

- **PON (National Operative Program**) titled 'IT@CHA-Tecnologie Italiane per applicazioni avanzate nei Beni Culturali' (IT@CHA-Italian Technologies for Advanced application in Cultural Heritage Assets')
Dr. Moliterni has been person in charge of the PON for the IC-CNR unit of Bari.
Period: 01/07/2011- 31/10/2015

- **SuperComputing Resource Allocation (ISCRA)** project class C, Title: 'Utilizing parallel computing for crystal structure solution from X-ray powder diffraction data (PSSPD)'
Period: 6 July, 2017 - 6 April, 2018
Hardware resources: Marconi KNL partition, CINECA.

- **MIUR-FIRB2011** titled 'Rete Integrata per la NanoMedicina (RINAME)'
Period: 22/02/2012-22/02/2016.

- **Progetto FIRB** - PROGRAMMA "FUTURO IN RICERCA", Titolo: Microtecnologie e moderne tecniche spettroscopiche e diffrattometriche per lo sviluppo e la razionalizzazione di processi di sintesi stereoselettivi ecosostenibili
Period: 01/12/2010 - 01/06/2014

Type of sector: Crystallography, Software development, Materials Science, ab-initio structure solution by single crystal and powder diffraction data, qualitative and quantitative phase analysis, Teaching Crystallography

November 1998 – February 2001

Researcher (full time/not permanent position)

Institute for the Development of Crystallographic Methodologies (IRMEC) - CNR
c/o Dipartimento Geomineralogico, Campus Universitario
Via Orabona, 4 - 70126 Bari – Italy

Main activities: Development of new methodologies aimed at improving the main steps of the *ab-initio* structure solution process (among them, the indexing process) and their implementation in crystallographic software. Structure solution by Direct Methods. Combined use of electron, X-ray and neutron diffraction data. Collection of X-ray diffraction data.

Type of sector: Crystallography, Software development, ab-initio structure solution by single crystal and powder data, X-ray diffraction experiments.

July 1997 – June 1998

Collaboration with IRMEC - CNR, Bari – Italy

Institute for the Development of Crystallographic Methodologies (IRMEC) - CNR
c/o Dipartimento Geomineralogico, Campus Universitario
Via Orabona, 4 - 70126 Bari – Italy

Aim of the collaboration: 'Trattamento di profili di diffrazione multifase da polveri finalizzato all'analisi qualitativa'.
Main activities: Contribution to the development of a Rietveld program for quantitative phase analysis, able to estimate the weight fraction of the crystalline phases in a polycrystalline mixture from powder diffraction data.

Type of sector: Crystallography, Software development, quantitative phase analysis by powder diffraction data

June 1996 - June 1997

Research Fellow at IRMEC - CNR, Bari - Italy
Competition Announcement n. 201.05.28 of 12/07/95 Code 21.05.04

Institute for the Development of Crystallographic Methodologies (IRMEC) - CNR
c/o Dipartimento Geomineralogico, Campus Universitario
Via Orabona, 4 - 70126 Bari – Italy

Main activities: Development of new methods for the treatment of powder diffraction data and the *ab-initio* structure solution of crystalline materials from powder diffraction data aimed at:

1) optimizing the software *EXTRA*, a program able to estimate the integrated intensities from a powder pattern;
2) contributing to develop the package *EXPO*, a program able to solve crystal structures from powder diffraction data.

Type of sector: Crystallography, Software development, ab-initio structure solution by powder diffraction data, full pattern decomposition process.

April 1996-June 1996

Collaboration with IRMEC - CNR, Bari - Italy

Institute for the Development of Crystallographic Methodologies (IRMEC) - CNR
c/o Dipartimento Geomineralogico, Campus Universitario
Via Orabona, 4 - 70126 Bari – Italy

Aim of the collaboration: 'Integrazione delle informazioni Patterson con Metodi Diretti'.
Main activities: Development of a new procedure based on the use of the prior information on the positivity of the Patterson map and aimed at improving the process of the integrated intensities estimation from a powder diffraction pattern, carried out by the software EXTRA. Implementation of the new procedure in crystallographic software.

Type of sector: Crystallography, Software development, ab-initio structure solution by powder diffraction data, full pattern decomposition process.

March 1995-February 1996

Research Fellow at IRMEC - CNR, Bari – Italy
Competition Announcement n. 201.19.1 of 11/30/94, Code 05.01.10

Institute for the Development of Crystallographic Methodologies (IRMEC) - CNR
c/o Dipartimento Geomineralogico, Campus Universitario
Via Orabona, 4 - 70126 Bari – Italy

Main activities: Development of new methods for the treatment of powder diffraction data and the *ab-initio* structure solution of crystalline materials from powder diffraction data. Implementation of the new procedures in crystallographic software.

Type of sector: Crystallography, Software development, ab-initio structure solution by powder diffraction data.

December 1992-November 1994

Research Fellow at IRMEC - CNR, Bari - Italy
Competition Announcement n. 224.05.4 of 12/31/91, Code 24.05.03

Institute for the Development of Crystallographic Methodologies (IRMEC) - CNR
c/o Dipartimento Geomineralogico, Campus Universitario
Via Orabona, 4 - 70126 Bari – Italy

Main activities: Development of new methods able to improve the phasing process by single crystal diffraction data. Implementation of the new procedures in crystallographic software.

Type of sector: Crystallography, Software development, ab-initio structure solution by single crystal diffraction data .

EDUCATION AND TRAINING

1-3 July, 2019

Eu-SPRI Summer school
'Tools and methods for analysing complex Science, Technology and Innovation (STI) systems: A gentle Introduction to Machine Learning (ML), Network Science (NS) and Text Mining (TM)'

Replace with EQF (or other) level if relevant

organized by IRCRES-CNR, Rome – Italy

- List of principal subjects covered or skills acquired:
  Basics on Machine Learning, Network Science, Text Mining.

9-11 May, 2000

Advanced Course:
'The Fortran for scientific computing'

Replace with EQF (or other) level if relevant

organized by CILEA, Segrate (MI) – Italy

- List of principal subjects covered or skills acquired:
  Advanced knowledge of Fortran, scientific computing.

December 1991

Degree in Physics (general address), University of Bari, mark of 110/110 *cum laude*

Replace with EQF (or other) level if relevant

Title: 'Generazione di radiazione laser in processi di 'scattering' Raman per applicazioni a diagnostiche in fase gassosa'

Dr. Moliterni has carried out the work of the Thesis at the Raman Spectroscopy and Remote Sensing Laboratories of the ENEA in Frascati (RM).

1985

Diploma, Scientific High School "Enrico Fermi" , Policoro (MT), mark of 60/60

Replace with EQF (or other) level if relevant

PERSONAL SKILLS

Mother tongue(s): Italian

Other language(s):
- Fluent spoken and written English.
- Fluent spoken and written French.

Job-related skills: Structure characterization of crystalline materials by single crystal and powder diffraction data; qualitative and quantitative phase analysis by powder diffraction data; software development

Digital skills

- **Programming language**: good knowledge of FORTRAN.
- **Operating systems**: good knowledge of Linux and Windows.
- **Other programming skills**: debugging, code optimization.

ADDITIONAL INFORMATION

Publications

Relevant publications*:

(*to be noted that for most of the papers listed below and published in the period 1995-2018, the order of the authors is alphabetic; this rule is not valid in the case of the latest papers, published from 2020 on):

Coriolano, A., **Moliterni, A.,** Todisco, F., Polimeno, L., Mastria, R., Olieric, V., Giacobbe, C., De Giorgi, M., Ballarini, D., Rizzo, A., Gigli, G., Giannini, C., Viola, I., Sanvitto, D., De Marco, L. **(2024).** 'Exploring structural and photophysical properties of Dion-Jacobson Perovskites and their use as Polariton Waveguides', *Adv. Mater.,* **Submitted.**
IF(2022) = 29.4

Mastria, R., Riisnaes, K.J., Bacon, A., Leontis, I., Lam, H.T., Saleh Alshehri, M.A., Colridge, D., Chan, T. H. E., De Sanctis, A., De Marco, L., Polimeno, L., Coriolano, A., Moliterni, A., Olieric, V., Giannini, C., Heppleston, S., Craciun, M. F., Russo, S. (**2024**). 'Real time and highly sensitive sub-wavelength 2D Hybrid perovskite photodetectors', *Adv. Mater.*, **Submitted**.
IF(2022) = 29.4

Bravetti, G., Taurisano, N., Moliterni, A., Vicent-Luna, J.M., Altamura, D., Aiello, F., Vanni, N., Capodilupo, A.L., Carallo, S., Gigli, G., Uccello-Barretta, G., Balzano, F., Giannini, C., Tao, S., Colella, S., Rizzo, A. (**2024**). 'Solution Aging Promotes the formation of Hexagonal Polytypes in Mixed Cation/-Halide Perovskites', *Chem. Mater.* **36**, 3150–3163.
DOI: doi.org/10.1021/acs.chemmater.3c02694
IF(2022) = 8.6 **Citations**: 0 **Source**: Web of Science

Balassone, G., Panikorovskii, T.L., Pellino, A., Bazai,A. V., Bocharov, V. N., Goychuk, O. F., Avdontseva, E. Y, Yakovenchuk, V.N., Krivovichev, S.V., Petti, C., Cappelletti, P., Mondillo, N., Moliterni, A., Altomare, A., Izzo, F. **(2024).** 'Enricofrancoite, $KNaCaSi_4O_{10}$, a new Ca-K-Na silicate from Somma-Vesuvius volcano, southern Italy'. *Miner. Magazine*, pp. 1-34, (Published online by Cambridge University Press: **26 February 2024)**
DOI: 10.1180/mgm2024.9
IF(2022) = 2.2 **Citations**: 0 **Source**: Web of Science

Quarta, D., Toso, S., Fieramosca, A., Dominici, L. Caliandro, R., **Moliterni, A.,** Tobaldi, D., Saleh, G., Infante, I., Cola, A., Giannini, C., Manna, L., Gigli, G., Giansante, C. **(2023).** 'Direct Band Gap Chalcohalide Semiconductors: Quaternary $AgBiSCl_2$ Nanocrystals', *Chem. Mater.* **35**, 9900–9906.
DOI: 10.1021/acs.chemmater.3c01403
IF(2022) = 8.6 **Citations**: 0 **Source**: Web of Science

Nakagawa, T., Ding, Y., Bu, K., Lü, X., Liu, H., Moliterni, A., Popovic, J., Mihalik, M.; Jaglicic, Z.; Mihalik, M.; Vrankić, M. (**2023**). 'Photophysical behaviour of triethylmethylammonium tetrabromoferrate(III) under high pressure', *Inorg. Chem*. **62**, 19527-19541.
DOI: 10.1021/acs.inorgchem.3c02607
IF(2022) = 4.6 **Citations**: 0 **Source**: Web of Science

Ray, A., Martín-García, B., Prato, M., **Moliterni, A**., Bordignon, S., Spirito, D., Marras, S., Goldoni, L., Boopathi, K. M., Moro, F., Casati, N., Giacobbe, C., Saidaminov, M., Giannini, C., Chierotti, M., Krahne, R., Manna, L., Abdelhady, A. **(2023).** 'Mixed organic cations promote ambient light-induced formation of metallic lead in lead halide perovskite crystals', *ACS Appl. Mater. Interfaces*, **15**, 28166–28174.
DOI: 10.1021/acsami.3c03366
IF(2022) = 9.5 **Citations**: 1 **Source**: Web of Science

Giacobbe, C., **Moliterni, A.,** Di Giuseppe, D., Malferrari, D., Wright, J. P., Mattioli, M., Ranieri, S., Giannini, C., Fornasini, L., Mugnaioli, E., Ballirano, P., Gualtieri, A. F. **(2023).** 'The Crystal structure of the killer fibre erionite from Tuzköy (Cappadocia, Turkey)', *IUCrJ* **10**, 397-410.

DOI: 10.1107/S2052252523003500
IF(2022) = 3.9 **Citations**: 1 **Source**: Web of Science

Quarta, D., Toso, S., Saleh, G., Caliandro, R. **Moliterni, A.,** Griesi, A., Divitini, G., Infante, I., Gigli, G., Giannini, C., Manna, L., Giansante, G. **(2023).** 'Mixed valence of Bismuth in Hexagonal Chalcohalide Nanocrystals', *Chem. Mater.* **35**(3), 1029-1036.
DOI: 10.1021/acs.chemmater.2c02941
IF(2022) = 8.6 **Citations**: 5 **Source**: Web of Science

Titi , A., Zaidi, K., Alzahrani, A. Y. A. El Kodadi, M., Yousfi, E. B., **Moliterni, A**., Hammouti, B., Touzani, R., Abboud, M. **(2023).** 'New In Situ Catalysts Based on Nitro Functional Pyrazole Derivatives and Copper (II) Salts for Promoting Oxidation of Catechol to o-Quinone', *Catalysts* **13**(1), 162.
DOI: 10.3390/catal13010162
IF(2022) = 3.9 **Citations**: 6 **Source**: Web of Science

Gassara, M., Msalmi, R., Lui, X., Hassen, F., **Moliterni, A**., Ben Hamadi, N., Guesmi, A., Khezami, L., Soltani, T., Naili, H. **(2022)**. 'A promising 1D Cd-based hybrid perovskite-type for white-light emission with high-color-rendering index', *RSC Adv*. **12**, 33516- 33524.
DOI: 10.1039/d2ra04676h
IF(2022) = 3.9 **Citations:** 5 **Source**: Web of Science

Titi, A., Touzani, R., **Moliterni, A.**, Ben Hadda, T., Messali, M., Benabbes, R., Berredjem, M., Bouzina, A., Al-Zaqri, N., Taleb, M., Zarrouk, A., Warad, I. **(2022).** 'Synthesis, structural, biocomputational modeling and antifungal activity of novel armed pyrazoles', *J. Mol. Struct*. **1264**, 133156.
DOI: 10.1016/j.molstruc.2022.133156
IF(2021) = 3.841 **Citations:** 14 **Source**: Web of Science

Titi, A., Touzani, R., **Moliterni, A.,** Giacobbe, C., Baldassarre, F., Taleb, M., Al-Zaqri, A., Zarrouk, A., Warad, I.: "Ultrasonic Clusterization Process to Prepare $[(NNCO)_6Co_4Cl_2]$ as a Novel Double-Open-Co_4O_6 Cubane Cluster: SXRD Interactions, DFT, Physicochemical, Thermal Behaviors, and Biomimicking of Catecholase Activity" **(2022).** *ACS Omega* **7**, 32949-32958.
DOI: 10.1021/acsomega.1c07032
IF(2022) = 4.1 **Citations**: 3 **Source**: Web of Science

Toso, S., Imran, M., Mugnaioli, E., **Moliterni, A.**, Caliandro, R., Schrenker, N.J., Pianetti, A., Zito, J., Zaccaria, F., Wu, Y., Gemmi, M., Giannini, C., Brovelli, S., Infante, I., Bals, S., Manna, L. **(2022),** 'Halide Perovskites as Disposable Epitaxial Templates for the Phase- Selective Synthesis of Lead Sulfochloride Nanocrystals', *Nat. Comm*. **13**, 3976.
DOI: 10.1038/s41467-022-31699-1
IF(2022) = 16.6 **Citations**: 16 **Source**: Web of Science

Quarta, D., Toso, S., Giannuzzi, R., Caliandro, R., **Moliterni, A**., Saleh, G., Capodilupo, A.L., Debellis, D., Prato, M., Nobile, C., Maiorano, V., Infante, I., Gigli, G., Giannini, C., Manna, L., Giansante, C. **(2022).** 'Colloidal Bismuth Chalcohalide Nanocrystals', *Angew. Chem. Int. Ed*. **61**, e202201747.
DOI: 10.1002/anie.202201747
IF(2022) = 16.6 **Citations**: 15 **Source**: Web of Science

Ray, A., Martín-García, B., **Moliterni, A.**, Casati, N., Boopathi, K. M., Spirito, D., Goldoni, L., Prato, M., Giacobbe, C., Giannini, C., Di Stasio, F. , Krahne, R., Manna, L., Abdelhady, A. L. **(2022).** 'Mixed Dimethylammonium/Methylammonium Lead Halide Perovskite Crystals for Improved Structural Stability and Enhanced Photodetection', *Adv. Mater*. **34**, Article Number: 2106160.
DOI:10.1002/adma.202106160.
IF(2022) = 29.4 **Citations**: 23 **Source**: Web of Science

Polimeno, L., Lerario, G., De Giorgi, M., De Marco, L., Dominici, L., Todisco, F., Coriolano, A., Ardizzone, V., Pugliese, M., Prontera, C. T., Maiorano, V., **Moliterni, A.,** Giannini, C., Olieric, V., Gigli, G., Ballarini, D., Xiong, Q., Fieramosca, A., Solnyshkov, D., Malpuech, G., Sanvitto, D. **(2021).** 'Tuning of the Berry curvature in 2D perovskite polaritons', *Nat. Nanotechnol*. **16**, 1349-1354.
DOI:10.1038/s41565-021-00977-2.
IF(2022) = 38.3 **Citations**: 30 **Source**: Web of Science

Cinquino, M., Fieramosca, A., Mastria, R., Polimeno, L., **Moliterni, A.,** Olieric, V., Matsugaki, N., Panico, R., De Giorgi, M., Gigli, G., Giannini, C., Rizzo, A., Sanvitto, D., De Marco, L. **(2021).** 'Managing Growth

And Dimensionality of Quasi 2D Perovskite Single-Crystalline Flakes For Tunable Excitons Orientation', *Adv. Mater*. **33**, 2102326.
DOI:10.1002/adma.02102326
IF(2022) = 29.4 **Citations**: 17 **Source**: Web of Science

Dhanabalan, B., Biffi, G., **Moliterni, A.,** Olieric, V., Giannini, C., Saleh, G., Ponet, L., Prato, M., Imran, M., Manna, L., Krahne, R., Artyukhin, S., Arciniegas, M. P. **(2021).** 'Engineering the Optical Emission and Robustness of Metal-Halide Layered Perovskites through Ligand Accommodation', *Adv. Mater*. **33**, 2008004.
DOI:10.1002/adma.202008004
IF(2022) = 29.4 **Citations**: 21 **Source**: Web of Science

Sayer, I., Dege, N., Ghalla, H., **Moliterni, A**., Naili, H. **(2021).** 'Crystal structure, DFT studies and thermal characterization of new luminescent stannate (IV) based inorganic-organic hybrid compound', *J. Mol*. *Struct*., **1224**, 129266.
DOI:10.1016/j.molstruc.2020.129266
IF(2022) = 3.8 **Citations**: 21 **Source**: Web of Science

Giacobbe, C., Di Giuseppe, D., Zoboli, A., Lassinantti Gualtieri, M., Bonasoni, P., **Moliterni, A.,** Corriero, N., Altomare, A., Wright, J., Gualtieri, A.F. **(2021).** 'Crystal structure determination of a lifelong biopersistent asbestos fibre using single-crystal synchrotron X-ray micro-diffraction', *IUCrJ* **8,** 76-86.
DOI:10.1107/S2052252520015079
IF(2022) = 3.9 **Citations**: 8 **Source**: Web of Science

Toso, S., Akkerman, Q.A., Martin-Garcia, B., Prato, M., Zito, J., Infante, I., Dang, Z., **Moliterni, A.**, Giannini, C., Bladt, E., Lobato, I., Ramade, J., Bals, S., Buha, J., Spirito, D., Mugnaioli, E., Gemmi, M., Manna, L. **(2020).** 'Nanocrystals of Lead Chalcohalides: A Series of Kinetically Trapped Metastable Nanostructures', *J. Am. Chem. Soc.* **142,** 10198-10211.
DOI: 10.1021/jacs.0c03577
IF(2022) = 15.0 **Citations**: 33 **Source**: Web of Science

Moliterni, A., Altamura, D., Lassandro, R., Olieric, V., Ferri, G., Cardarelli, F., Camposeo, A., Pisignano, D., Anthony, J.E., Giannini, C. **(2020).** 'Synthesis, crystal structure, polymorphism and microscopic luminescence properties of anthracene derivate compounds', *Acta Cryst. B* **76,** 427-435.
DOI:10.1107/S2052520620004424
IF(2022) = 1.9 **Citations**: 9 **Source**: Web of Science

Cinquino, M., Polimeno, L., Lerario, G., De Giorgi, M., **Moliterni, A.,** Olieric, V., Fieramosca, A., Carallo, S., Mastria, R., Ardizzone, V., Dominici, L., Ballarini, D., Giannini, C., Sanvitto, D., Rizzo, A., De Marco, L. **(2020).** 'One-Step Synthesis at Room Temperature of Low Dimensional Perovskite Single Crystals with High Optical Quality', *J. Lumin*. **221**, 117079.
DOI: 10.1016/j.jlumin.2020.117079
IF(2022) = 3.6 **Citations**: 10 **Source**: Web of Science

Altomare, A., Corriero, N., Cuocci, C., Falcicchio, A., **Moliterni, A.,** Rizzi, R. **(2018).** 'OChemDb: the free online Open Chemistry Database portal for searching and analysing crystal structure information', *J. Appl. Cryst*. **51**, 1229-1236.
DOI: 10.1107/S1600576718008166
IF(2022) = 6.1 **Citations**: 9 **Source**: Web of Science

Altomare, A., Corriero, N., Cuocci, C., Falcicchio, A., **Moliterni, A.,** Rizzi, R. **(2017).** 'Main features of QUALX2.0 software for qualitative phase analysis', *Powder Diffraction*, 32(S1), S129-S134.
DOI:10.1017/S0885715617000240
IF(2022) = 0.5 **Citations**: 11 **Source**: Web of Science

Valant, M., Popovic, J., Mihelj, M.V., Burazer, S., Altomare, A., **Moliterni, A. (2017).** 'Oxide Crystal Structure with Square-Pyramidally Coordinated Vanadium for Integrated Electronics Manufactured at Ultralow Processing Temperatures', *ACS Sustainable Chem. Eng*. **5**, 5662-5668.
DOI: 10.1021/acssuschemeng.6b03111
IF(2022) = 8.4 **Citations**: 5 **Source**: Web of Science

Altomare, A., Corriero, N., Cuocci, C., Falcicchio, A., **Moliterni, A.,** Rizzi, R. **(2015).** *'QUALX2.0*: A qualitative phase analysis software using the freely available database POW_COD', *J. Appl. Cryst*. **48**, 598-603.
DOI:10.1107/S1600576715002319
IF(2022) = 6.1 **Citations**: 204 **Source**: Web of Science

Salomone, A., Perna, F.M., Falcicchio, A., Lill, S. O. N., **Moliterni, A**., Michel, R., Florio, S., Stalke, D., Capriati, V. **(2014).** 'Direct observation of a lithiated oxirane: a synergistic study using spectroscopic, crystallographic, and theoretical methods on the structure and stereodynamics of lithiated ortho-trifluoromethyl styrene oxide', *Chem. Sci*. **5**, 528-538.
DOI: 10.1039/c3sc52099d
IF(2022) = 8.4 **Citations**: 46 **Source**: Web of Science

Altomare, A., Cuocci, C., Giacovazzo, C., **Moliterni, A.,** Rizzi, R.; Corriero, N., Falcicchio, A. **(2013).** 'EXPO2013: A kit of tools for phasing crystal structures from powder data', *J. Appl. Cryst.* **46**(4), 1231-1235.
DOI: 10.1107/S0021889813013113
IF(2022) = 6.1 **Citations**: 677 **Source**: Web of Science

de Ceglie, M. C., Musio, B., Affortunato, F., **Moliterni, A.**, Altomare, A., Florio, S., Luisi, R. **(2011).** 'Solvent- and Temperature-Dependent Functionalization of Enantioenriched Aziridines', *Chem. Eur. J*. **17**, 286-296.
DOI: 10.1002/chem.201002172
IF(2022) = 4.3 **Citations**: 37 **Source**: Web of Science

Altomare, A., Camalli, M., Cuocci, C., Giacovazzo, C., **Moliterni, A.,** Rizzi, R. **(2009).** *'EXPO2009*: Structure solution by powder data in direct and reciprocal space', *J. Appl. Cryst*. **42**, 1197-1202.
DOI: 10.1107/S0021889809042915
IF(2022) = 6.1 **Citations**: 265 **Source**: Web of Science

Altomare, A., Campi, G., Cuocci, C., Eriksson, L., Giacovazzo, C., **Moliterni, A.,** Rizzi, R. & Werner, P.-E. **(2009).** 'Advances in powder diffraction pattern indexing: *N-TREOR09'*, *J. Appl. Cryst*. **42**, 768-775.
DOI: 10.1107/S0021889809025503
IF(2022) = 6.1 **Citations**: 109 **Source**: Web of Science

Altomare, A., Cuocci, C., Giacovazzo, C., **Moliterni, A.,** Rizzi, R. **(2008).** QUALX: a computer program for qualitative analysis using powder diffraction data', *J. Appl. Cryst*. **41**, 815-817.
DOI:10.1107/S0021889808016956
IF(2022) = 6.1 **Citations**: 51 **Source**: Web of Science

Altomare, A., Cuocci, C., Giacovazzo, C., Kamel, G. S., **Moliterni, A**., Rizzi, R. **(2008).** 'Minimally resolution biased electron-density maps', *Acta Cryst. A***64**, 326-336.
DOI: 10.1107/S0108767308004303
IF(2022) = 1.8 **Citations**: 29 **Source**: Web of Science

Altomare, A., Caliandro, R., Cuocci, C., Giacovazzo, C., **Moliterni, A.G.G**., Rizzi, R., Platteau, C. **(2008).** 'Direct methods and simulated annealing: A hybrid approach for powder diffraction data', *J. Appl. Cryst.* **41**, 56-61.
DOI: 10.1107/S0021889807054192
IF(2022) = 6.1 **Citations**: 31 **Source**: Web of Science

Altomare, A., Caliandro, R., Camalli, M., Cuocci, C., da Silva, I., Giacovazzo, C., **Moliterni, A.G.G**., Spagna, R. **(2004).** 'Space-group determination from powder diffraction data: A probabilistic approach', *J. Appl. Cryst*. **37**, 957-966.
DOI: 10.1107/S0021889804023982
IF(2022) = 6.1 **Citations**: 41 **Source**: Web of Science

Altomare, A., Caliandro, R., Camalli, M., Cuocci, C., Giacovazzo, C., **Moliterni, A.G.G**., Rizzi, R. **(2004).** 'Automatic structure determination from powder data with EXPO2004', *J. Appl. Cryst*. **37**, 1025-1028.
DOI :10.1107/S0021889804021417
IF(2022) = 6.1 **Citations**: 182 **Source**: Web of Science

Margiotta, N., Bertolasi, V., Capitelli, F., Maresca, L., **Moliterni, A.G.G.**, Vizza, F., Natile, G. (**2004).** 'Influence of steric and electronic factors in the stabilization of five-coordinate ethylene complexes of platinum(II): X-ray crystal structure of [PtCl2(2,9-dimethyl-1,10-phenanthroline-5,6-dione)]', *Inorganica Chimica Acta*, **357**, 149-158.
DOI:10.1016/S0020-1693(03)00382-7
IF(2022) = 2.8 **Citations**: 32 **Source**: Web of Science

Harcharras, M., Capitelli, F., Ennaciri, A., Brouzi, K., **Moliterni, A.G.G.**, Mattei, G., Bertolasi, V. **(2003).** 'Synthesis, X-ray crystal structure and vibrational spectroscopy of the acidic pyrophosphate

KMg0.5H2P2O7·H2O', *J. Solid State Chem.*, **176**, 27-32.
DOI:10.1016/S0022-4596(03)00339-6
IF(2022) = 3.3 **Citations**: 33 **Source**: Web of Science

Altomare, A., Burla, M. C., Giacovazzo, C., Guagliardi, A., **Moliterni, A.G.G**. Polidori, G., Rizzi, R. **(2001).** 'Quanto: a Rietveld program for quantitative phase analysis of polycrystalline mixtures'*, J. Appl. Cryst*. **34**, 392-397.
DOI: 10.1107/S0021889801002904
IF(2022) = 6.1 **Citations**: 102 **Source**: Web of Science

Altomare, A., Giacovazzo, C., Guagliardi, A., **Moliterni, A.G.G.,** Rizzi, R., Werner, P.-E. **(2000).** 'New techniques for indexing: N-TREOR in EXPO', *J. Appl. Cryst*. **33**, 1180-1186.
DOI: 10.1107/S0021889800006427
IF(2022) = 6.1 **Citations**: 173 **Source**: Web of Science

Altomare, A., Giacovazzo, C., Guagliardi, A., **Moliterni, A.G.G**., Rizzi, R. **(1999).** 'Solving crystal structures from powder data. V. Located molecular fragment and powder-pattern decomposition', *J. Appl. Cryst*. **32**, 963-967.
DOI: 10.1107/S0021889899007165
IF(2022) = 6.1 **Citations**: 59 **Source**: Web of Science

Altomare, A., Burla, M. C., Camalli, M., Carrozzini, B., Cascarano, G. L., Giacovazzo, C., Guagliardi, A., **Moliterni, A.G.G.,** Polidori, G., Rizzi, R. **(1999).** *'EXPO*: a program for full powder pattern decomposition and crystal structure solution', *J. Appl. Cryst*. **32**, 339-340.
DOI: 10.1107/S0021889898007729
IF(2022) = 6.1 **Citations**: 441 **Source**: Web of Science

Altomare, A., Burla, M. C., Camalli, M., Cascarano, G. L., Giacovazzo, C., Guagliardi, A., **Moliterni, A.G.G.,** Polidori, G. Spagna, R. **(1999).** *'SIR97*: a new tool for crystal structure determination and refinement', *J. Appl. Cryst*. **32**, 115-119.
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