PERSONAL INFORMATION Anna Moliterni

Institute of Crystallography - National Research Council
Via Amendola, 122/O
70126 Bari - Italy

(+39) 080 5929156 (

annagrazia.moliterni@ic.cnr.it

Sex Female | *Date of birth* _ | *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.
  Her expertise 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, 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 her research activity 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 is documented by:

- **Bibliometric parameters (July, 2023):**
  ISI Web of Knowledge source:
  Overall number of publications: **146** documents, H-index = **27**; Sum of Times Cited (Without self citations): **> 12850**, Citing articles (Without self citations) **> 12250**;

Scopus source:
Overall number of publications: **118**documents, H-index = **24**; number of citations (Without self citations) **> 12800,** Co-authors: **about 250.**

- **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/).

- **CNR award:**
On October 1, 2009, she 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*'.

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

- **Patent:**
Co-invertor on a 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).

- **Organization of International Schools, Chairing Teaching Activities and Commissions;**

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

- **Role of 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(2022)=5.5, ISSN = 2296-2646.

- **Member of the Editorial Board** of the MDPI journal Crystals [IF(2022)=2.7, ISSN=2073-4352].

- **Member of Editors of the Special Issue of Crystals** [IF(2022)=2.7, 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

- Most Recent Research Projects:

- **PRIN 2022 - DDG decreto direttoriale n. 104 del 2 febbraio 2022 - Project related to *Macrosettore Physical Sciences and Engineering – PE5 Synthetic Chemistry and Materials***
  Project title: Conjugated organic-inorganic two-dimensional halide perovskite for stable solar cells and modules (CONPER)- Project code: **2022CBBEHN**
  Duration: 24 months, Approval date: 22/06/2023 (Decreto Direttoriale n. 926 del 22/06/2023 https://www.mur.gov.it/it/atti-e-normativa/decreto-direttoriale-n-926-del-22-6-2023
  https://www.mur.gov.it/sites/default/files/2023-06/Decreto%20Direttoriale%20n.%20926%20del%2022-6-2023%20-%20PE5_AllegatoB.pdf
  https://www.mur.gov.it/sites/default/files/2023-06/Decreto%20Direttoriale%20n.%20926%20del%2022-6-2023%20-%20PE5_AllegatoA.pdf)
  Funds MUR: €: 201,887,00
  Principal Investigator (PI): Prof. Aldo Di Carlo

- **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, Funded for €: 80.000,00

- **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.
  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*
  Period: 01/09/2022 – 31/08/2025

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.

Collaboration with IRMEC - CNR, Bari – Italy

July 1997 – June 1998

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)'
organized by IRCRES-CNR, Rome – Italy

Replace with EQF (or other) level if relevant

- 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'
organized by CILEA, Segrate (MI) – Italy

Replace with EQF (or other) level if relevant

- 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'
The work of the Thesis has been carried out 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

Date: July, 18 2023