

## CONTACTS

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## WEB

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## QUALIFICATIONS

- Materials Science  
with focus on Nano-Materials
- Scattering Methods  
with focus on Powder X-ray Diffraction
- Atomistic Simulations
- Scientific Computing, Large Data Analysis
- Mathematical Modelling, Virtual Experiments
- Software Development, Programming

## SOFT SKILLS

### Interpersonal

- Critical Thinker
- Problem Solving
- Team Player
- Accepting Constructive Critics

### Transversal

- Leading Projects
- Advising & Mentoring Students
- Teaching & Proofing Methodology
- Responsible Conduct of Research

## MEMBERSHIPS & AFFILIATIONS

- **ICDD Member | 2020-present**  
International Center for Diffraction Data
- **FAU-CBI Habilitands Board | 2019-present**  
Friedrich-Alexander University (Germany)
- **IU Research Affiliate | 2017-present**  
Indiana University Bloomington - IN (USA)
- **Italian body of Engineers | 2010-present**
- **Departmental Board | 2009-2012**  
Representative of Ph.D. students  
University of Trento (Italy)

## HONORS

- **Best Graduate Student | 2007**  
Faculty of Engineering - University of Trento)

# Alberto Leonardi | Ph.D.

## SUMMARY

Experienced in Computational Materials Science and Materials Characterization via Scattering Methods. I study nano-structured materials for energy and sustainability applications. I combine experimental with simulation methods to link in-situ observations with mechanical models of materials. Excellent ability to work independently and as a team. Effective in multidisciplinary activities. Able to present highly technical material in a clear and concise manner. Highly focused to learn about innovative topics.

## WORK EXPERIENCE

### Postdoctoral Scientist | 2020-present

UKRI-STFC - ISIS Neutron and Muon Source (United Kingdom)

- Research in the fields of scattering methods, and kinetics of formation and transformation of crystals
- Support for users of the SXD single crystal diffractometer at ISIS
- Coordination of feasibility studies and liaison with external networks and facilities
- Development of HPC applications for multi-scale simulation and data analysis
- Leading projects, advising students
- Writing grant proposals

### Postdoctoral Research Associate | 2017-2020

Friedrich-Alexander University Erlangen-Nuremberg (Germany)

- Research in the fields of powder scattering, catalysis and kinetics of formation of crystal structures
- Development of HPC applications for multi-scale simulation and data analysis
- Lecturing academic courses in the subject of "Simulation of Granular and Molecular Systems"
- Leading projects, advising students
- Writing grant proposals

### Postdoctoral Research Associate | 2015-present (formal affiliation since 2017)

Indiana University Bloomington (USA)

- Research in the fields of powder X-ray diffraction and layered nano-materials
- Development of HPC applications for multi-scale simulation and data analysis
- Leading projects, advising students

### Postdoctoral Research Fellow | 2013-2014

University of Trento (Italy)

- Research in the fields of powder X-ray diffraction, and single-crystal and polycrystalline nano-materials
- Development of HPC applications for multi-scale simulation and data analysis
- Leading projects, advising students
- Writing grant proposals

### Philosophical Doctorate | 2008-2012

University of Trento (Italy)

- Research in the fields of powder X-ray diffraction and molecular dynamics simulations
- Development of HPC applications for multi-scale simulation and data analysis
- Leading projects, advising students

### Teacher | AYs 2007/2008, 2008/2009, 2012/2013

High-School G. Floriani - Riva del Garda (Italy)

- Solid Mechanics
- Materials Science
- Worksite Safety

### Engineer | 2007-2008

Civil Engineering s.r.l. - Arco (Italy)

- Research in the field of building sustainability
- Urban and building planning

## EDUCATION

### Accademic Habilitation | 2019 - present (expected end of program 2023)

Friedrich-Alexander University Erlangen-Nuremberg (Germany)

### Master's Degree - Education | July 2013

University of Padova (Italy)

### Doctorate of Philosophy - Materials Science and Engineering | November 2012

University of Trento (Italy)

### Master's Degree - Civil Engineering and Architecture | March 2007

University of Trento (Italy)

## LANGUAGES

- **Italian**  
Native Speaker
  - **English**  
Professional Working Proficiency
  - **German**  
Elementary
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## CERTIFICATIONS

- **License to Teach** (High-School Grade)  
University of Padova (Italy)
  - **License to Practice Engineering**  
University of Trento (Italy)
  - **License to Practice Architecture**  
IUAV University of Venice (Italy)
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## INSTRUMENT EXPERIENCE

- **RAL - ISIS Neutron and Muon Source (UK)**  
SXD
- **Argonne National Laboratory (USA)**  
APS - 11BM
- **Elettra Sincrotrone Trieste (Italy)**  
MCX
- **In-House**  
Bruker D8 Powder Diffractometer

## HPC EXPERIENCE

### SCARF - United Kingdom

Scientific Computing Application Resource for Facilities

### RRZE - Germany

Regionales RechenZentrum Erlangen

- Emmy Cluster
- Woody Cluster

### UITS - USA

University Information Technology Services

- Karst
- Big-Red II
- Big-Red III
- Big-Red 200

### UNITN - Italy

University of Trento

- CISCA Cluster
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## TEACHING

### Friedrich-Alexander University Erlangen-Nuremberg (Germany)

- AY 2020/21 fall semester | Simulation of Granular and Molecular Systems (student evaluation available)
- AY 2019/20 fall semester | Simulation of Granular and Molecular Systems (student evaluation available)
- AY 2017/18 fall semester | Basics in Computational Materials Science

### High-School G. Floriani - Riva del Garda (Italy)

- AY 2012/13 | Solid Mechanics, Materials Science, Worksite Safety
  - AY 2008/09 | Solid Mechanics, Materials Science
  - AY 2007/08 | Solid Mechanics, Materials Science
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## STUDENT

### 2020

- **Mentor for the "ARIADNE Mentoring-Program for high-potential female students"**
- Master student **miniproject**,  
Zeair Omar
- Master student - Soft Matter **Journal Club**,  
Kamm Lukas

### 2019

- Master student **miniproject**,  
Chou Chun-Yu
  - Master student - Soft Matter **Journal Club**,  
Dominick Martens
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## GRANT

### 2020

- **DFG self-standing grant** (Germany)
- **DFG-NSF** (Germany - USA) as co-PI
- **KONWIHR** (Germany)
- **EAM-Finanzierung** (Germany)

### 2019

- **DFG** (Germany)
  - **KONWIHR** (Germany)
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## PARTICIPATION

### 2020

- **Oral** | USA | 69th DXC  
Annual Denver X-ray Conference

### 2019

- **Invited Lecture** | Germany | CBI Symposium
- **Oral** | Germany | ISAM4  
4th International Symposium on Atomistic,  
Multiscale Modeling of Mechanics
- Poster | Germany | PBM19  
Particle-Based Materials Symposium
- **Oral** | France | Euroclay 2019

### 2018

- **Oral & Poster** | Germany | MSE18  
Materials Science Engineering
- **Oral** | Germany | PBM18  
Particle-Based Materials Symposium

### 2017

- Posters (2) | USA | MRS Fall-Meeting 2017  
Materials Research Society
- Poster | Germany | PBM17  
Particle-Based Materials Symposium
- Poster | Germany | ICEAM17  
International Conference  
Engineering Advanced Materials
- Poster | Spain | ICC17  
16th International Clay Conference

### 2016

- Poster | Italy | EPDIC15  
15th European Powder Diffraction Conference
- Poster | USA | Clay Mineral Society  
53rd Annual Meeting

### 2018

- Master student **miniproject** review,  
Chou, Chun-Yu
- Master student **internship**,  
Levine Valerie

### 2017

- Master student **miniproject**,  
Chen Liu

### 2015

- **Master student thesis**,  
Amimi Amine
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### 2017

- **ETI** - Emerging Talent Initiative (Germany)

### 2014

- **SIR** self-standing grant (Italy)
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### 2015

- **Invited Lecture** | UK | 7th Size Strain
- Poster | UK | Euroclay 2015
- Poster | Italy | DSE15  
Debye Scattering Equation Conference

### 2014

- **Invited Lecture** | Germany | Materials Science  
Colloquium
- **Oral** | Italy | Workshop NANO
- Poster | Denmark | EPDIC14  
14th European Powder Diffraction Conference

### 2013

- **Invited Lecture** | UK | ECM28  
European Crystallographic Meeting

### 2012

- Posters | France | EPDIC13  
13th European Powder Diffraction Conference

### 2011

- **Oral** | Italy  
Advanced Computational Methods Workshop
- **Oral** | France | 6th Size strain
- Posters | Germany | 2nd International Workshop on  
the Plasticity of Nanocrystalline Metals
- Posters | France | E-MRS Spring-Meeting 2011

### 2010

- Posters | Germany | EPDIC12  
12th European Powder Diffraction Conference

## JOURNAL COVER

• Acta Crystallographica 72 | 2016

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## PUBLICATION

- \* **IUCrJ – 8 (2021) 257**  
*Whole Pair Distribution function Modeling: the Bridging of Bragg and Debye Scattering Theories*
- Nature Communication – 11 (2020) 3041**  
*Imaging the kinetics of anisotropic dissolution of bimetallic core-shell nanocubes*
- Nanoscale Advances – 2 (2020) 1105**  
*Effect of Lattice Mismatch and Shell Thickness on Strain in Core@Shell Nanocrystals*
- \* **Inorganic Chemistry – 59 (2020) 5357**  
*Understanding Powder X-ray Diffraction Profiles from Layered Minerals: The Case of Kaolinite Nanocrystals*
- ACS Nano – 13 (2019) – 4008**  
*Achieving Highly Durable Random Alloy Nanocatalysts through Intermetallic Cores*
- \* **ACS Nano – 12 (2018) 9186**  
*Particle Shape Control via Etching of Core@Shell Nanocrystals*
- \* **Acta Materialia – 133 (2017) 380**  
*Interactions of lattice distortion fields in nano polycrystalline materials revealed by molecular dynamics and X-ray powder diffraction*
- Journal of Applied Crystallography – 50 (2017) 508**  
*Debye-Waller coefficient of heavily deformed nanocrystalline iron*
- \* **Journal of Applied Crystallography – 49 (2016) 1593**  
*High-performance powder diffraction pattern simulation for large-scale atomistic models via full-precision pair distribution function computation*
- Scientific Reports – 6 (2016) 20712**  
*On the reliability of powder diffraction Line Profile Analysis of plastically deformed nanocrystalline systems*
- Physical Review B – 91 (2015) 155414**  
*Anisotropic atom displacement in Pd nanocubes resolved by molecular dynamics simulations supported by x-ray diffraction imaging*
- Journal of Applied Crystallography – 48 (2015) 1534**  
*Structure and morphology of shape-controlled Pd nanocrystals*
- \* **Metallurgical and Materials Transactions A 47 (2015) 5722**  
*Dislocation Effects on the Diffraction Line Profiles from Nanocrystalline Domains*
- \* **Journal of Applied Physics – 117 (2015) 164304**  
*Eshelby twist and correlation effects in diffraction from nanocrystals*
- \* **Frontiers in Materials – 1 (2015) 37**  
*Atomistic model of metal nanocrystals with line defects: contribution to diffraction line profile*
- \* **LAMBERT Academic Publishing (2013) ISBN: 978-3-659-40764-2**  
*Molecular Dynamics and X-ray Powder Diffraction Simulations*
- \* **Journal of Applied Crystallography – 46 (2013) 63**  
*Directional Pair Distribution Function for Diffraction Line Profile Analysis of Atomistic Models*
- \* **Thin Solid Films – 530 (2013) 40**  
*Atomistic interpretation of microstrain in Diffraction Line Profile Analysis*
- \* **Powder Diffraction – 28 S2 (2013) S184**  
*Diffraction line broadening from nanocrystals under large hydrostatic pressures*
- \* **Computational Materials Science – 67 (2013) 238**  
*Atomistic modelling of polycrystalline microstructures: an evolutionary approach to overcome topological restrictions*
- \* **Philosophical Magazine – 92 (2012) 986**  
*Realistic nano-polycrystalline microstructures: beyond the classical Voronoi Tessellation*
- \* **University of Trento (2012) ISBN: 978-88-8443-455-5**  
*Molecular Dynamics and X-ray Powder Diffraction Simulations: "investigation of nano-polycrystalline microstructure at the atomic scale coupling local structure configurations and X-ray powder diffraction techniques"*
- \* **Journal of Nanoscience & Nanotechnology 12 (2012) 8546**  
*Strain in atomistic models of nanocrystalline clusters*
- \* **Metallurgical and Materials Transactions A 44 (2012) 39**  
*Interference effects in nanocrystalline systems*
- \* **Journal of Applied Crystallography – 45 (2012) 1162**  
*Common Volume Functions and Diffraction Line Profiles of polyhedral domains*
- \* **Zeitschrift für Kristallographie Proceeding - I (2011) 37**  
*Microstrain in nanocrystalline samples from atomistic simulation*

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\* first author