

Curriculum Vitae - Ana Belén Muñoz García

Name/Surname: Ana Belén / Muñoz García (She/Her)

Born: July 27th 1981 in Madrid, Spain

E-mail: anabelen.munozgarcia@unina.it

Marital status: Married, 1 daughter

ACADEMIC TRACK

- 12/2017- 05/2021 **Associate Professor**
University of Naples Federico II (Italy)
Department of Physics “Ettore Pancini”
- 12/2017- 05/2021 **Assistant Professor (RTD-B)**
University of Naples Federico II (Italy)
Department of Physics “Ettore Pancini”
- 10/04/2017 **National Scientific Habilitation (ASN 2016)**
Associate Professorship (II Fascia) - 03/A2
Models and Methodologies for Chemical Sciences
- 09/2012- 09/2017 **Assistant Professor (RTD-A)**
University of Naples Federico II (Italy)
Department of Chemical Sciences

RESEARCH EXPERIENCES AND EDUCATION

- 04/2011 – 04/2012 **Postdoctoral Research Associate (1 year)**
Princeton University (USA), Department of Mechanical and
Aerospace Engineering - Prof. Emily A. Carter group
- 11-12/2010 **Visiting Research Scholar (1 month)**
Princeton University (USA), Department of Mechanical and
Aerospace Engineering - Prof. Emily A. Carter group
- 05-08/2010 **Visiting Student Research Collaborator (3 months)**
Princeton University (USA), Department of Mechanical and
Aerospace Engineering - Prof. Emily A. Carter group
- 01-04/2008 **Visiting Research Scholar (3 months)**
University of Cambridge (UK), Department of Earth Sciences Prof.
Emilio Artacho group
- 10/2006 – 03/2011 **Ph.D. student (4 years)**
Universidad Autónoma de Madrid (Spain)
Supervisor: Prof. Luis Seijo. Thesis: “*First-principles studies on Ce-doped YAG: codoping, antisite defects and Ce 4f–5d transitions*”
- 06/2006 **M.Sc. degree in Chemistry**

Universidad Autónoma de Madrid (Spain), with Honors

BIBLIOMETRICS (as of 16/12/2021)

Articles in peer-reviewed scientific journals: **71**
- as corresponding author: **14**

Total citations	1933 (Scopus)	2234 (Google Scholar)
h-index	27 (Scopus)	29 (Google Scholar)
i10-index		46 (Google Scholar)

First article published in 2009 (academic age 12 years)

Scopus profile: <https://www.scopus.com/authid/detail.uri?authorId=26667032600>

Google Scholar profile: <https://scholar.google.it/citations?user=olv6pCUAAA&hl=en>

SELECTED INVITED LECTURES AND SEMINARS

- ***Defective but effective: the role of defects in oxide-based electrocatalysts***^{[1][2]}
Materials Research Society (MRS) Fall Meeting & Exhibition, Boston, USA - 2/12/2019
- ***Computational study of carbon dioxide photoreduction to methanol on copper-iron delafossite***
Congress: *Solar driven chemistry: towards new catalytic solutions for a sustainable world*. Accademia dei Lincei, Rome (Italy), 18/10/2018 – Invited Poster and Presentation
- ***Design of Heterogeneous Functional Materials for Energy Conversion Devices: a Quantum-Chemical Perspective***
Ecole Normale Supérieure de Lyon – Lyon, France. 07/04/2018. Invited Seminar.
- ***First-Principles Design of Mixed Proton-Electron Conductors for Solid-Oxide Fuel Cell Electrodes***
Giornate Elettrochimica Italiana 2018 – Sestriere, Italy. 23/01/2018 . Invited Speaker
- ***Computational modeling of solid-state materials: from energy applications to cultural heritage***
Department of Civil & Environmental Engineering, Massachusetts Institute of Technology, Boston, USA.
09/03/2016. Invited Seminar.
- ***Complex materials for energy conversion: some things we can learn from Quantum Mechanics***
Department of Materials Sciences and Engineering, Technion, Haifa, Israel.
06/07/2015. Invited Seminar.
- ***Heterogeneous materials for energy conversion: what can we learn from Quantum Mechanics?***

Departamento de Química Inorgánica, Orgánica y Bioquímica, Universidad de Castilla-La Mancha, Ciudad Real, Spain, 03/10/2014. Invited Seminar

- ***Oxygen Transport in Perovskite-Type Materials for SOFCs Cathodes: What Can We Learn from Quantum Mechanics?***

225th Meeting of The ElectroChemical Society, Orlando, USA. 14/05/2014. Keynote Speaker.

- ***Elucidation of materials properties from first-principles calculations: oxygen transport in perovskite-type materials for SOFC applications.***

Scuola Normale Superiore di Pisa, Italia. 24/01/2014. Invited Seminar

- ***Unveiling structure-property relationships in perovskite oxides based electrodes for solid oxide fuel cell applications.***

Ecole Nationale Supérieure de Chimie de Paris, Francia. 11/12/2012. Invited Seminar.

ACTIVITY IN THE SCIENTIFIC COMMUNITY

- **>20 oral contributions** to international and national meetings

- Affiliated to the **Società Chimica Italiana, American Chemical Society, Materials Research Society** and **ElectroChemical Society**

- **EU-COST Action member:** PERSPECT-H₂O *Supramolecular Photocatalytic Water Splitting*

- **EU-COST Action member:** CA18234 *Computational materials sciences for efficient water splitting with nanocrystals from abundant elements*

- **Referee** for the following international peer-reviewed journals:

Journal of the American Chemical Society, Physical Chemistry Chemical Physics, Angewandte Chemie International Edition, Energy & Environmental Science, Chemical Science, Journal of Materials Chemistry A, Journal of Physical Chemistry A/B/C, Journal of the Electrochemical Society, RSC Advances, Chemical Communications, Catalysis Science & Technology, Computational Materials Sciences, New Journal of Chemistry, Materials Science in Semiconductor Processing, Journals of Alloys and Compounds, J. Inorg. Org. Polymers and Materials, Materials Chemistry and Physics, Energy Storage Materials, ACS Applied Materials and Interfaces, J. Power. Sources, ACS Energy Letters, ACS Crystal Growth & Design, Physica Status Solidi, Journal of Molecular Structure

AWARDS & RECOGNITIONS

- Selected as **Emerging Investigator 2020** by *Physical Chemistry Chemical Physics*

- **Front Cover** of article: R. Mori, G. Iasilli, M. Lessi, A. B. Muñoz-García, M. Pavone, F. Bellina, *Luminescent solar concentrators based on PMMA films obtained from a red-emitting ATRP initiator.* *Polym. Chem.*, 2018, **9**, 1168-1177¹_{SEP} (Front Cover Vol. 9, Issue 10, 14/03/2018)

- **Front Cover** of article: C. Huang, A.B. Muñoz-García, M. Pavone *Effective scheme for partitioning covalent bonds in density-functional embedding theory: From molecules to*

extended covalent systems J. Chem. Phys., 145, 244103, 2016^{[1][1]} (Front Cover Vol. 145, Issue 24, 28 December 2016)

- **Interview and Highlight** on Royal Society of Chemistry magazine *Chemistry World: Unstable dyes to blame for Van Gogh's waning Sunflowers* - 04/04/2016^{[1][1]}
- **Highlight of article:** A.B. Muñoz-García and E.A. Carter, *Non-Innocent Dissociation of H₂O on GaP(110): Implications for Electrochemical Reduction of CO₂* J. Am. Chem. Soc. 134, 13600- 13603, 2012 in Editor's *Spotlights on Recent JACS Publications* (J. Am. Chem. Soc. 134, 15163, 2012)
- **Lucio Senatore Award 2015**, 1st European Conference on Physical and Theoretical Chemistry, Best Poster of the Physical Chemistry Division
- **Personal Investigador en Formación 2007-2011**^{[1][1]} Nationally Competitive Graduate Ph.D. Fellowships
- **Premio Especial de Fin de Carrera 2006**^{[1][1]} Highest GPA Award Universidad Autónoma de Madrid
- **Beca de Aprovechamiento Académico Excelente 2004, 2005**^{[1][1]} Regional Competitive Undergraduate fellowships for students with high marks record, Universidad Autónoma de Madrid

PARTICIPATION TO RESEARCH PROJECTS

- **Principal Investigator (PI)**
Computational Characterization of chemico-physical properties of electrode materials for perovskite solar cells.
MISE-ENEA PTR 2019-2021. Funding: euro 140.000
- **Principal Investigator (PI)**
Perovskite Oxide Electrode-Solvent Interaction: an Ab-Initio Study - POESIAS
ISCRA-CINECA High performance computing Grant 2013 (500.000,00 CPU hours - 1 year)
- **As a member of a Research Unit**

2011-2012 USA- DoD-MURI "Novel catalytic Mechanisms for the Chemical Reduction of Carbon dioxide to Energy-Dense Liquids" (AFOSR Award No. FA9550-10-1-057) (PI: Prof. Emily A. Carter):
responsible of the studies on heterogeneous catalysis at GaP/H₂O interface

2010-2012 USA- DoE-EFRC 2010-2012 "Heterogeneous Functional Materials: HeteroFoaM" (Basic Energy Sciences Award No DE-SC0001061) (PI: Prof. Emily A. Carter): responsible of the characterization of new catalysts for solid oxide fuel cells

- 2013-2016 IT - Progetto FIRB Futuro in Ricerca 2012 "Design of nano-heterogeneous materials for solar energy conversion" (RBFR122HFZ). Member of UNINA Research Unit (PI: Prof. Michele Pavone): responsible of the work package devoted to p-type electrodes for dye sensitized solar cells
- 2014-2017 Progetto PRIN 2012 "Theoretical study of hybrid organic-inorganic materials in complex chemical environments" (2012NB3KLK). Member of UNINA Research Unit (PI: Prof. Michele Pavone): responsible of the work package devoted to modeling processes at electrode-molecule interfaces
- 2017-2020 Progetto PRIN 2015 "Towards quantum-photovoltaics: ultrafast energy and charge transport in hybrid nanomaterials" (2015XBZ5YA_006). Member of UNINA Research Unit (PI: Prof. Michele Pavone): responsible of the work package devoted to modeling charge and energy transfer processes at solid organic-inorganic interfaces in model nanoparticle-molecule devices.

TEACHING & MENTORING ACTIVITY

Responsible for the following courses:

- **Chemistry** (6CFU) – Department of Physics "Ettore Pancini"
B.Sc. Physics
AY: 2018/2019, 2019/2020, 2020/2021
- **Physical Chemistry of Materials** (6CFU) – Department of Chemical Sciences
M.Sc. Industrial Chemistry
AY: 2013/2014, 2014/2015, 2015/2016, 2016/2017, 2018/2019, 2019/2020, 2020/2021
- **Electronic Structure of Solid-State Materials** (6CFU) – Department of Chemical Sciences
PhD. School in Chemical Sciences
AY: 2012/2013, 2013/2014, 2014/2015, 2015/2016, 2016/2017, 2017/2018, 2018/2019, 2019/2020, 2020/2021

Advisor of:

- 2 Ph. D Student in Chemical Sciences
- 13 M.Sc Thesis in Chemical Sciences
- 7 B.Sc Thesis in Chemistry
- 3 M.Sc Thesis in Science and Technology of Industrial Chemistry
- 9 B.Sc Thesis in Industrial Chemistry

Member of the Faculty Board

Ph.D. School in Astrochemistry - Scuola Normale Superiore di Pisa
AY 2018/2019, 2019/2020, 2020/2021