Curriculum Vitae

Personal information

First name(s) / Surname	**Maria Barbara Maccioni**
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Google Scholar	https://scholar.google.it/citations?user=9lBwTX4AAAAJ&hl=en
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Professional Topics, Interests And Skills

Topics	Multiferroicity, Self-assembled monolayers (SAMs), adsorption mechanism on surfaces, Magnetic molecules for quantum computing.
Interests	Simulations, through DFT approach, of electronic structure and magnetic properties in multiferroic materials, wide-gap and polar oxides, influence of doping on the structural and electronic properties in order to increase the catalytic performance of oxides, chemical functionalization of semiconductors, adsorption of molecules on surfaces.
Technical skills	• Ab-initio Simulation programs: • VASP (Vienna Ab initio Simulation Package) • Quantum Espresso with D3q and Thermal2 suites • Quantum Espresso with Koopmans package • Phonopy • AlmaBTE
Computer skills and competences	• Unix-based OS: Linux, Ubuntu, Mac OS, Windows 10/8/7/ XP/2000 • Packages: Office, OpenOffice, LibreOffice • Engineering math software: Mathcad • Markup language: LaTeX
Data analysis and visualization:	• Origin • VESTA • XCrySDen • Materials Studio

Professional Experiences

Research Activities

2023 – present	**Post-doc research fellow**
Title of project	*"Computational modelling (by ab initio techniques) of molecular and crystalline systems with strong couplings between magnetic, structural and transport properties"*
Supervisor	Prof. Matteo Cococcioni Department of Physics, University of Pavia
2019 – 2021	**Post-doc research fellow**
Title of project	"*Simulation of passivation schemes for germanium surfaces and nanostructures for nanoelectronics"*
Supervisor	Dr. Michael Nolan Tyndall National Institute, University College Cork

2017 – 2018	**Post-doc research fellow (Borsa di ricerca)**
Title of project	"*Ab initio study of multiferroics for thermoelectric applications*"
Supervisor	Prof. Vincenzo Fiorentini Department of Physics, University of Cagliari

Didactic Activities

2017	**Tutor** in the – *General Physics II course* at Department of Engineering – *Physics course* at Department of Medical Sciences – *Physics course* at Department of Chemical and Geological Sciences – *Physics and scientific Method course* at Department of Mathematics and Computer Science – *High School Teachers Upgrade course in Quantum Mechanics* at Department of Physics University of Cagliari **Tutor online** in the – *General Physics II course* at Department of Engineering, e-learning University of Cagliari **Teacher** in the – *Orientation course for High School Students* at Department of Physics University of Cagliari
2016	**Tutor** in the – *Physics course* at Department of Natural Science – *General Physics II course* at Department of Engineering University of Cagliari **Tutor online** in the – *General Physics II course* at Department of Engineering, e-learning University of Cagliari
From 2013 to 2015	**Tutor** in the – *General Physics II course* at Department of Engineering University of Cagliari

Education

18/03/2016	**Ph.D in Physics** University of Cagliari, Department of Physics
Title of thesis	"*Magnetoelectric, multiferroic, wide-gap, and polar oxides for advanced applications: first-principles theoretical studies*"
Supervisor	Prof. Vincenzo Fiorentini
Sector	Computational Physics of Condensed Matter
Principal subjects/occupational skills covered	Simulations, through DFT approach, of electronic structure and magnetic properties in multiferroic materials, wide-gap and polar oxides.

23/02/2012	**Degree in Physics** University of Cagliari, Department of Physics
Title of thesis	"*Multiferroicity and magnetoelectricity of topological ferroelectric material*"
Supervisor	Prof. Vincenzo Fiorentini

Principal subjects/occupational skills covered	Research activity on computational physics, study of phase transitions, polarization and magnetic order in a particular perovskite layered, with Ab initio simulation program: VASP

Lifelong Learning Activities

International schools

9-11 November 2022	"Advanced Quantum ESPRESSO tutorial: Hubbard and Koopmans functionals from linear response" Virtual tutorial
06-15 August 2013	School on "Density Functional Theory and Beyond: Computational Materials Science for Real Materials", Trieste, Italy
15-19 July 2013	School on "Electronic structure at the cutting edge with Elk", Lausanne, Switzerland

Badges and Certificates

2020	**Certificate "Publons Academy Peer Reviewer"**
Issued by	Publons Academy
2020	**Digital Badge in "Postgraduate Research Supervision"**
Issued by	National Forum for the Enhancement of Teaching and Learning in Higher Education, University College Cork, Ireland

Development Activities and Professional Training Courses

2020

Tyndall Training & Development Programme:

- *Unconscious Bias Training Course*
- *Introduction to Social Media (Beginner)*
- *Time Management & Personal Effectiveness*
- *Introduction to the suite of EU*

Tyndall National Institute, University College Cork (Ireland)

ERC- Development group

- ERC- Training Tyndall- *Preparation budget*
- ERC- Training Tyndall- *CV Clinic*
- ERC- Training Tyndall- *Writing with impact*
- ERC- Training Tyndall- *The importance of policy in research proposal writing*

Tyndall National Institute, University College Cork (Ireland)

UCC Professional Skills for Research Leaders (RSS):

- *Presentation skills for Research Staff*
- *Applying for funding – Panel discussion with evaluators*
- *Proposal writing*
- *Addressing Dissemination, Communication and Outreach in Research Proposals*
- *Impact*
- *F.A.I.R. Research Data Management*

University College Cork - Cork (Ireland)

UCC On-Line Sessions for Research Staff:

- *Transitioning to a Leadership Role & Different Leadership Styles*
- *Career Planning for you & Listening to your Team*
- *Managing a Research Team*
- *How to prepare a Non-Academic CV*

- *Planning for a Career beyond Academia*
- *Interview Skills*
- *Mentoring*
- *Commercial Awareness and Knowledge Transfer*
- *Sourcing and Accessing Non-Academic Career Opportunities*
- *Innovation and Entrepreneurship*
- *Leading a Research Team*

University College Cork - Cork (Ireland)

General training

- *LEAD (Living Equality and Diversity e-Learning Programme) online training*
- *Scopus Research Metrics & Indicators* training
- *Scopus hands-on workshop*
- *Web of Science training*
- *Research Integrity Epigeum (Concise)*
- *Research Supervisor Training*
- *Writing and preparing a journal article for publication*
- *Publons Academy: peer review training course*
- *UCC RSS Workshop-Getting ready for Horizon Europe*
- *SFI_HBR_Wellcome Research partnership*

University College Cork - Cork (Ireland)

Conferences, Meetings and Workshops

06-10 June 2016	"13th ETSF Young Researchers' Meeting", King's College London, London, UK
14-15 July 2014	"5th Young Researcher Meeting in Trieste", SISSA, Trieste, Italy
16-18 June 2014	"SiO_2-Advanced Dielectrics and Related Devices 2014", Cagliari, Italy
09-13 September 2013	"FISMAT2013 - Italian National Conference on Condensed Matter Physics (Including Optics, Photonics, Liquids, Soft Matter)", Milano, Italy
06- 15 August 2013	"Density Functional Theory and Beyond: Computational Materials Science for Real Materials", ICTP, Trieste, Italy
15-19 July 2013	"Electronic structure at the cutting edge with Elk", Lausanne, Switzerland
20- 23 May 2013	"MAMA-Trend: Trends, challenges and emergent new phenomena in multi-functional materials", Sorrento, Italy

Grants

Grants at the *Irish Centre for High-End Computing* (ICHEC) for allocation of computer time on High-Performance Computing (HPC).

2020	"First Principles Modelling of Germanium Surfaces and Nanostructures for Nanoelectronics"
Budget	1M standard hours (Class B project)
2020	"First Principles Modelling of Germanium Surface Functionalization with Hydrophobic Polymer Chains"
Budget	100K standard hours (Class C project)
2019	"First Principles Modelling of Germanium Surface Functionalized with Organic Chains for Molecular Doping"
Budget	100K standard hours (Class C project)

Grants at the *Italian Super-Computing Resource Allocation* (ISCRA) for allocation of computer time on high-performance computing (HPC) systems operated by CINECA **(**nonprofit Consortium of Italian universities and institutions - http://www.hpc.cineca.it)

2023	CITRUS – **"**moleCular rIng magneTs foR qUantum technologieS**"**
Budget	30K standard hours
2018	K-LATIO – **"**Ab initio thermal conductivity of a layered perovskite, $La_2Ti_2O_7$**"**
Budget	30K standard hours
2017	THERMO – **"**Ab initio study of multiferroics for thermoelectric applications**"**
Budget	50K standard hours
2016	EPS-GAOX – **"**First-principles study of the structural, electronic, and magnetic properties of epsilon- Ga_2O_3 alloys**"**
Budget	12.5K standard hours
2015	INGAOX – **"**Structure and band offsets in the small-x $In_2O_3/(Ga_{1-x}In_x)_2O_3$ system**"**
Budget	25K standard hours
2014	GAOX – **"**First-principles study of the structural, electronic, and thermodynamic properties of Ga_2O_3 alloys**"**
Budget	50K standard hours

Last update 2023