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Marco Di Gennaro

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ABOUT ME

With 15 years of experience among corporate, SMEs and academic, my R&D activity sits at the edge between materials science and machine learning. I specialise in energy storage, spintronic materials, and computational simulation enhancements through quantum computing and AI. My leadership at Atomistic Modelling has steered pioneering research in materials for decarbonisation, notably in battery electrolytes and nano-materials for H2 production and storage, directly supporting sustainable energy solutions.

My expertise and collaborative projects resonate with the EU's priorities in climate, defence, health, and food security, showcasing my capacity to contribute significantly to these domains. My background aligns with the EU's strategic goals, demonstrating a commitment to leveraging advanced materials for a sustainable and secure future.

WORK EXPERIENCE

01/07/2023 – CURRENT Bruxelles, Belgium

FOUNDER & FREELANCE CONSULTANT ATOMISTIC MODELLING

- Established a SME specialised in machine learning & materials simulation
- Derived data-driven models in material research for energy applications
- Managed operations and strategic planning, financial strategies
- Cultivated partnerships within industrial and academic sectorr
- Analytical and numerical techniques to extract insight in automotive
- Associated Partner in the *EUSpecLab*: ML techniques for spectroscopy

Business or Sector Professional, scientific and technical activities | **Email** mdg@atomistic-modelling.com |

Website https://atomistic-modelling.com/

01/06/2018 – 28/02/2023 Brussels, Belgium

MACHINE LEARNING SCIENTIST TOYOTA MOTOR EUROPE & KLANIK SA

- Materials Research and Development (R & D): Led the integration of multiscale simulations and machine learning multi-disciplinary nano-materials research
- Operational Data Management Efficiency: Streamlined data operations, boosting team productivity and enhancing project communication underlying the innovativeness of data-driven approach
- Strategic Research and Development: Directed strategic research initiatives, employing Toyota's management principles to foster innovation and operational safety
- Quantum Computing for Materials: Pioneered the use of quantum computing in material optimisation project

- Team Development and Mentorship: Participated in the recruitment process and professional training of students in Python and AI, enhancing team capabilities
- Grant Management and Training: Successfully managed EU grant acquisition and delivered comprehensive training programs in machine learning

01/12/2015 – CURRENT Liege, Belgium
SCIENTIFIC COLLABORATOR LIEGE UNIVERSITY

- First-Principles Modelling Innovation: Drove the advancement in the study of fundamental interactions affecting material properties
- Spin Caloritronics Analysis: Provided new insights into temperature-dependent material behaviours, developing predictive models
- Computational Material Science: Expertise in harmonising theoretical predictions with experimental data
- Grant Management: Demonstrated proficiency in securing and managing EU research grants

01/01/2021 – 06/2021 Corato, Italy
PROJECT MANAGER PIN BIKE

- EU Initiative Leadership: Successfully spearheaded and won a competitive EU urban mobility initiative, overseeing budget negotiations and partnership agreements
- Team Recruitment and Leadership: Played a pivotal role in the selection and recruitment of a results-driven communication team, ensuring effective project dissemination

01/09/2017 – 18/12/2017 Los Angeles, United States
INVITED FELLOW INSTITUTE OF PURE AND APPLIED MATHEMATICS | UCLA

Applied Mathematical Research: Engaged in complex energy landscape research, contributing to the field of applied mathematics and encouraged scientific, Multi-disciplinary team work

01/08/2016 – 31/05/2018 Basel, Switzerland
RESEARCH ASSISTANT UNIVERSITY OF BASEL

- Materials Informatics Management: Committed to the accurate application of materials data in various projects, bridging team communication gaps
- Project Coordination and Flexibility: Coordinated team efforts effectively, managing multiple projects with a focus on strategic prioritisation

Business or Sector Professional, scientific and technical activities | **Department** Chemistry department |

Website https://chemspacelab.chem.utoronto.ca/

EDUCATION AND TRAINING

15/03/2011 – 01/09/2015 Liege, Belgium
PHD Liege University

Website https://www.uliege.be/

01/09/2008 – 09/09/2010 Bari, Italy
MS IN THEORETICAL PHYSICS Bari University

Website https://www.uniba.it

01/09/2005 – 18/12/2008 Bari, Italy
BS IN THEORETICAL PHYSICS Bari University

Website https://www.uniba.it

LANGUAGE SKILLS

Mother tongue(s): **ITALIAN**

Other language(s):

	UNDERSTANDING		SPEAKING		WRITING
	Listening	Reading	Spoken production	Spoken interaction	
ENGLISH	C1	C1	C1	C1	C1
FRENCH	C1	C1	C1	C1	C1
SPANISH	B1	B1	B1	B1	B1
GERMAN	A2	A2	A2	A2	A2
PORTUGUESE	A1	A1	A1	A1	A1
DUTCH	A1	A1	A1	A1	A1

Levels: A1 and A2: Basic user; B1 and B2: Independent user; C1 and C2: Proficient user

DIGITAL SKILLS

Linux (Terminal Commands, Bash/Shell) | Machine learning | High Performance Computing | Python | Workflows Engineering | ETL | Pandas | Numpy | Python, Scikit-Learn, Numpy, Matplotlib | Pytorch,Tensorflow

ADDITIONAL INFORMATION

COMMUNICATION AND INTERPERSONAL SKILLS

Communication Expertise: Bridging Academia and Industry into a multilingual context My journey from academia to the corporate sector has refined my communication skills, enabling me to distill complex concepts for diverse audiences effectively. With a strong foundation in presenting at international conferences, writing grants, and engaging with stakeholders, I excel at making technical information accessible to both experts and non-specialists. My proficiency in Italian, English, and French enhances my ability to connect and communicate across cultural boundaries, fostering collaboration and understanding in multinational environments.

CONFERENCES AND SEMINARS

15/03/2015 – 20/03/2015 – Berlin
Spring meeting of the German Physical Society Contributed talk: *Pure spin thermocurrent in Permalloy at high temperatures*

23/09/2014 – 26/09/2014 – Zaragoza
19th ETSF Workshop on Electronic Excitations: " Complex systems in Biology and Nanoscience" Contributed talk: Ab-initio calculation of Seebeck and spin-dependent Seebeck effects in metals

12/05/2014 – 16/05/2014
11th ETSF Young Researchers Meeting Contributed talk:*Seebeck, spin dependent Seebeck and spin Seebeck effect - an ab-initio approach*

07/04/2014 – 08/04/2014 – Berlin
ETSF - electron phonon coupling workshop: "From polarons to heat currents" Contributed talk: *Seebeck, spin dependent Seebeck and spin Seebeck effect - an ab-initio ap- proach*

20/12/2012 – Bari
3rd Bari Xmas theory workshop Contributed talk: *Spin orbit torques at the Ni-Pt interface - Ab-initio vs. tight binding*

20/05/2013 – 24/05/2013 – Budapest
10th ETSF Young Researchers Meeting
- Contributed talk:*The role of anharmonicity in the ab-initio phase diagram of calcium*
- Poster: *Ab-initio study of the Spin Seebeck effect in metallic alloys*

13/05/2013 – 16/05/2013 – Columbus, OH (USA)
Spin-Caloritronics V Poster: *Ab-initio study of the Spin Seebeck effect in metallic alloys*

18/03/2013 – 22/03/2013 – Baltimore, MD (USA)
American Physical Society march meeting 2013 Contributed talk: *The role of anharmonicity in the* ab-initio *phase diagram of calcium*

20/12/2012 – Bari
2nd Bari Xmas theory workshop Contributed talk: *The role of anharmonicity in the* ab-initio *phase diagram of calcium*

03/12/2012 – 06/12/2012 – Bonn
Spin-orbit-driven transverse transport phenomena Poster: Ab-initio study of the Spin Seebeck effect in metallic alloys

01/10/2012 – 06/10/2012 – Coimbra
17th ETSF Workshop on Electronic Excitations: "Advanced Green function methods" Poster: *The role of anharmonicity in the ab-initio phase diagram of calcium*

26/08/2012 – 29/08/2012 – Uppsala
SCAILD Workshop Contributed talk: *The role of anharmonicity in the* ab-initio *phase diagram of calcium*

21/05/2012 – 25/05/2012 – Bruxelles
9th ETSF Young Researchers Meeting Poster: *The role of anharmonicity in the* ab-initio *phase diagram of calcium*

07/05/2012 – 10/05/2012 – Cheshire
PSI-K research conference: Computational oxide spintronics Poster: *Ab-initio study of the Spin Seebeck effect in metallic alloys*

16/12/2011 – Bari
1st Bari Xmas theory Workshop Contributed talk: *Ab-initio calculations in condensed matter*

25/05/2011 – Namur
General meeting of the Belgian Physical Society

09/08/2011 – 12/08/2011 – Seggauerberg
ETSF electron-phonon coupling workshop

27/09/2011 – 30/09/2011 – Turin
16th ETSF Workshop on Electronic Excitations: "Bridging theory and experiment"

DRIVING LICENCE

Driving Licence: B | 22/04/2015 – 01/12/2025

HOBBIES AND INTERESTS

Ultimate frisbee, rock climbing

Social dance: Lindy Hop

Outdoor activities: bicycling, hiking

Language tandem

Chess

HONOURS AND AWARDS

01/09/2011
Personal PhD grant – FNRS-FRIA Ab-initio calculation of spin dependent transport quantities in disordered materials

01/09/2017
Invited Fellow – Institute of Pure and Applied Mathematics | UCLA

Link https://www.ipam.ucla.edu/programs/long-programs/complex-high-dimensional-energy-landscapes/

PUBLICATIONS

Ab initio calculation of thermoelectric properties in 3d ferromagnets based on spin-dependent electron–phonon coupling
– 2023

New J. Phys. 2023, 25 043022

1,2,3-Trimethoxypropane: a bio-sourced glyme as electrolyte for lithium–O2 batteries – 2022

Green Chem., 2022,24, 6016-6025

A combination of multi-scale calculations with machine learning for investigating hydrogen storage in metal organic frameworks Author links open overlay panel
– 2021

Int. J. Hydrog 021, 27612, 2021

Thermoelectric properties of elemental metals from first-principles electron-phonon coupling – 2020

Phys. Rev. B 102, 155128

Competition of lattice and spin excitations in the temperature dependence of spin-wave properties
– 2018

Phys. Rev. B 97, 214417

Complex Energy Landscapes – 2017

IPAM Whitepaper - 2017

Recent developments in the ABINIT software package – 2016

Role of Dynamical Instability in the Ab Initio Phase Diagram of Calcium

Phys. Rev. Lett. 111, 025503

PROJECTS

01/09/2022 – CURRENT
ML for Spectroscopy
- Application of ML Canonical Sampling in MoSx bi-layer materials
- Application of DNN methods to predict IR spectra of Cu clusters
- ML interatomic potentials for transport quantities of Si nanolayer

01/09/2022 – CURRENT
Battery materials
- Electrothermal simulations to understand battery stack for automotive
- Transport properties of Li-based electrolysers by MD and ML models
- Benchmark of ML Interatomic Potentials and classical force fields
- Active learning model to predict leakage in polymeric electrolysers

01/09/2021 – CURRENT
Fuel cells
- Application-driven material design for thermodynamical H2 storage
- Developed a suite of workflows to submit and query generic simulations
- Simulated ~1M nano-structures for room temperature absorption
- Computational pipeline to simulate ~150k Metal Organic Framework
- Feature Selection & Genetic Algorithm for H2 adsorption into crystals
- Calculated stress-strain resistance of carbon nano tubes and enhanced resistance with cross-functional linking for high pressure H2 storage
- Post DFT methods to design semiconductor for water photo-catalysis

01/09/2021 – 01/09/2023
Gas exhaust catalysis Clustering model to translate over 1M chemical hydrocarbon reactions into simplified (5-10), efficient model for human analysis

01/06/2018 – 01/09/2023

Lubricants

- Explained tribological macroscopic effects from molecular interactions
- Benchmark of several physics-inspired ML models, Feature Selection

Energy Landscapes

- Bayesian optimisation for fast geometry optimisation in DFT
- DCNN recognition of molecular interaction from electronic structure

01/08/2016 – 31/05/2018

NCCR MARVEL

- Machine Learning of electronic-structure materials properties
- QMAT-X: a reference database for crystallographic Machine Learning
- Feature Analysis and Algorithms benchmark (KRR, RF) for Quantum ML

Spin-Caloritronics materials

- Ab-initio study of electron–phonon coupling in metals
- Temperature dependence of spin-wave propagation stiffness
- Interaction model of magnetic and vibrational properties in materials

01/09/2011 – 31/12/2015

The ABINIT software package

- Collaborated with a global team to an open-source software package
- Alternative algorithm to parallelise independent phonon calculations
- Analysis and verification to ensure versions consistency

01/03/2011 – 31/12/2011

High-pressure phase transitions

01/03/2010 – 01/09/2010

Spin Glasses for frustrated systems