

MARCO DI GENNARO | PHD

Freelance Data Scientist with >10 years of R&D experience

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WORK EXPERIENCE

Founder & Freelance consultant Mar 2023 – Present
Atom | Bruxelles (Be)

- 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 sectors
- Analytical and numerical techniques to extract insight in automotive
- Associated Partner in the EUSpecLab: ML techniques for spectroscopy

Machine Learning Scientist Jun 2018 – May 2023
Toyota Motor Europe | Bruxelles (Be)

- Integrated simulations and machine learning in nano-materials research
- Delivered data-driven decision-making in multidisciplinary research projects
- Directed strategic research initiatives, employing Toyota's principles
- Developed and distributed several python packages for materials science
- Delivered training programs in python and machine learning
- Demonstrated the use of quantum computing in material science
- Demonstrated proficiency in securing and managing EU/HPC resources
- Participated in the recruitment process and training of students

Freelance Project Manager EU Projects Jan 2021 – Jun 2021
Pin Bike | Corato (It)

- Bicification EIT urban mobility project: pitch competition, budget negotiations (~€300K), partnership agreements and recruitment.

Invited Fellow Sep 2017 – Dec 2020
IPAM - UCLA | Los Angeles (USA)

- Long research program: Complex High-Dimensional Energy Landscapes
- Engaged in applied mathematics & multi-disciplinary team work

Research Assistant Aug 2016 – May 2018
University of Basel | Basel (CH)

- Integrated theoretical chemistry and machine learning
- Managed multiple projects with a focus on strategic prioritisation
- Organising Committee: The 2017 Basel Postdoctoral Network Retreat

Scientific Collaborator Sep 2015 – Dec 2022
University of Liege | Liege (Be)

- Provided new insights into temperature-dependent material behaviour

PhD Student (FRIA-FNRS personal grant) Mar 2011 – Aug 2015
Liège University - Nanomat | Liege (Be)

- Project management: running research grant of €10k over 4 years
- Research in computational solid state physics: Quantum transport, Spintronics, nano-devices, modelling of complex phenomena
- Visiting student at The University of Texas at Austin (USA)

HARD SKILLS

R&D Big Data Machine Learning
AI B2B Pipelines Data Science
Algorithms Modelling Data Analysis
Statistical Analysis ETL EDA
Data Visualisation Optimisation
High Performance Computing
Software Development Python
Pandas Numpy Scipy Pydantic
ScikitLearn Neural Networks
C++ Bash Databases MongoDB
SQL Git & Version Control CI/CD
Cloud Computing GCP AWS
Multiscale Simulations DFT MD
Monte Carlo Quantum Computing
Time Series Analysis Forecasting
Computer Vision Numerical Methods
Energy Materials Automotive

SOFT SKILLS

Dynamic Target oriented Flexible
Analytical thinking Problem solving
Attention to details Team work
Abstraction Passion Commitment
Supervision Reliable Leadership
Time Management Communication
Rigorous Versatile Storytelling
Divuligation Proof of Concepts

LANGUAGES

Italian - Native
English
French
Spanish
German
Dutch
Portuguese

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PROJECTS

ML for Spectroscopy | Atom & EUSpecLab Sep 2022 – Feb 2024

- Application of ML Canonical Sampling in MoS_x bi-layer materials
- Application of DNN methods to predict IR spectra of Cu clusters
- ML interatomic potentials for transport quantities of Si nanolayers

Batteries | Toyota Motor Europe & Atom Sep 2020 – Feb 2024

- Electrothermal simulations to understand battery stack for automotive
- Transport properties of Li-O₂ electrolyzers by MD and ML models
- Benchmark of ML Interatomic Potentials and classical force fields
- Active Learning prediction of polymeric electrolyzers degradation

Fuel cells | Toyota Motor Europe & Atom Sep 2019 – Feb 2024

- Application-driven material design for thermodynamical H₂ storage
- Developed a suite of workflows to manage vast amount of simulations
- Simulated ~1M nano-structures for room temperature absorption
- Computational pipeline to simulate ~150k Metal Organic Frameworks
- 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

Gas exhaust catalysis | Toyota Motor Europe Sep 2021 – Sep 2023

- Clustering model to translate over 1M chemical hydrocarbon reactions into simplified (5-10), efficient model for human analysis

Lubricants | Toyota Motor Europe Jun 2018 – Aug 2021

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

Energy Landscapes | IPAM Sep 2017 – Dec 2020

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

NCCR MARVEL | UBasel Aug 2016 – May 2018

- 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 | ULiege Sep 2011 – Apr 2020

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

The ABINIT software package | ULiege Sep 2011 – Dec 2015

- Collaborated with a global team to an open-source software package
- Parallelisation of phonon calculations on independent k-points
- Analysis and verification to ensure versions consistency




High-pressure phase transitions | ULiege Mar 2011 – Dec 2011

- Explained unusual crystallographic phase transition of Calcium via DFT

Spin Glasses for frustrated systems | UBari Mar 2010 – Sep 2010

- Analytical method to calculate free energy of frustrated systems

REFEREES

- Dr. Konstantinos Gkagkas 
Manager, Toyota Motor Europe
- Prof. Anatole von Lilienfeld 
Lab head: [Chemspacelab](#)
- Prof. Matthieu Verstraete 
Ph.D. supervisor, ULiege
Lab head: [Nanomate](#)

CERTIFICATES

- Introduction to MongoDB 2020
- Linux admin 2019
- Introduction to SQL 2018

PUBLICATIONS

1. New Journal of Physics **25**, 2023
2. Green Chem. **24**, 2022
3. Int. J. Hydrog **021**, 27612, 2021
4. Phys. Rev. B **102**, 155128, 2020
5. Phys. Rev. B **97**, 214417, 2018
6. Complex Energy Landscapes, 2017
7. Com. Phys. Comm. **205**, 106, 2016
8. Phys. Rev. Lett. **111**, 2013

EDUCATION

- PhD Computational Physics 2015
Liege University (Be)
- Visiting PhD student 2013
Austin University (TX/USA)
- MS Theoretical Physics 2010
Bari University (It)
- BS General Physics 2008
Bari University (It)
- Erasmus project 2008
Sorbonne University/CNRS (Fr)
- Liceo scientifico 2005
Ruvo di Puglia (It)

AWARDS

- Finalist MT180 2015
- FWB travel research grant 2013
- FRIA research fellowship 2011
- MS Committee award 2010

LEISURES ACTIVITIES

- Ultimate frisbee, rock climbing
- Social dance: Lindy Hop
- Outdoor activities: bicycling, hiking
- Language tandem, Chess