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
- Artificial Intelligence: sentiment analysis through LLM
  Wind power production through ML Renewables energy optimization
- 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 · Divulgation · Proof of Concepts

LANGUAGES

Italian - Native ●●●●●
English ●●●●●
French ●●●●●
Spanish ●●●○○
German ●●○○○
Dutch ●○○○○
Portuguese ●○○○○

PROJECTS

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

Batteries | Toyota Motor Europe & Atom Sep 2020 – Feb 2024
- Electrothermal simulations to understand battery stack for automotive
- Transport properties of Li-O2 electrolysers by MD and ML models
- Benchmark of ML Interatomic Potentials and classical force fields
- Active Learning prediction of polymeric electrolysers degradation

Fuel cells | Toyota Motor Europe & Atom Sep 2019 – Feb 2024
- Application-driven material design for thermodynamical H_2 storage
- Developed a suite of workflows to manage vast amount of simulations
- Simulated $\sim$1M nano-structures for room temperature absorption
- Computational pipeline to simulate $\sim$150k Metal Organic Frameworks
- Feature Selection & Genetic Algorithm for H_2 adsorption into crystals
- Calculated stress-strain resistance of carbon nano tubes and enhanced resistance with cross-functional linking for high pressure H_2 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: Nanomat

CERTIFICATES

- Quantum Computing 2024
- 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