MARCO DI GENNARO

Materials Science + Data Science = Materials Informatics | Ph.D.

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GOALS

- Be the edge between research, technology and digital innovation
- Achieve effective application-driven materials design
- Energy functional materials, carbon-negative materials
- Sustainable mobility solutions

EXPERTISE

- Materials simulation and multiscale modelling
- Machine learning: explore the Chemical Compound Space
- High performance calculation
- Project Management

DISTINCTIVE SKILLS

- **Project Management:**
  - > connecting multidisciplinar, technical know-how to business context
  - > translating data into decision to contribute to the big picture
  - > aking initiative and ownership of key points of industrial R&D process
  - > implementing large scale data solution for real-world applications
- **Science**: Mathematics, Physics, Chemistry, Statistics
- **Complex systems modelling**: effective interactions and toy models; multiscale parametrisation and coarse graining techniques; frustrated and disordered systems
- **Theoretical materials science:**
  - > quantum chemistry, density functional theory, semi empirical potentials, molecular dynamics, Monte Carlo
  - > Softwares: Gamess, Orca, Tutbomol, Abinit, Vasp, Lammps, Gromacs
- **Materials informatics**:
  - > Managing tools: aiida, ase, atomate, pymatgen, Python/C++ parsers
  - > Quantum and molecular descriptors
  - > High-throughput automatic algorithms for massive parallel calculations.
  - > Workload managers: sge, slurm
- **Machine learning**:
  - > optimisation techniques, clustering, classification and regression. Linear, polynomial and kernel methods. Neural networks and deep learning. Genetic and evolutionary algorithms
  - > big data: database construction, manipulation and visualisation. Query languages, pandas, json, csv
- **Quantum chemistry on quantum devices**: annealing and gate architectures. Algorithms and libraries for electronic calculations and molecular properties

MOST PROUD OF

IPAM invited fellow	2017
Finalist MT180	2015
FWB travel research grant	2013
FRIA research fellowship	2011
MS Committee award	2010

IT SKILLS

Windows, Mac, Unix	●●●●●
Office Suite	●●●●●
Bash/Command line	●●●●●
Python	●●●●●
LaTeX	●●●●●
Linux Admin	●●●●○
Git & Version control	●●●●○
Scikit-Learn	●●●●○
Keras	●●●○○
MongoDB & SQL	●●●○○
Mathematica	●●●○○
Matlab	●●●○○
C++	●●●○○

SOFT SKILLS

Curiosity | Time management
Creativity | Scientific writing
Teamwork | Problem solving
Adaptability | Critical thinking
Communication | Divulgation
Public speaking | Storytelling
Skepticism | Perseverance
Intellectual honesty | Passion
Result Oriented | Business sense

EXPERIENCE

Consultant — 2018 – Present
Klanik — Bruxelles (Be)

- **Toyota Motors Europe** Advanced Materials Research, R&D.
- **Project management:**
  - > Application-driven, inverse material design
  - > Bridging multiscale simulations through machine learning
  - > Coarse grained models and data-driven decisions
  - > Industrial and academic collaborations
- **Materials research for energy applications:** from quantum to mesoscale
  - > Lubricants: ionic liquids modelling and simulation, transport coefficients.
  - > H_2 adsorption and storage: Metal Organic Frameworks, Kubas adsorption, polymers for fuel cells membranes in GDL.
  - > Micromagnetic machine learning for materials cost reduction
  - > Quantum computing of molecular properties
  - > Catalysis: ab-initio photo-catalysis, mesoscale chemistry models
  - > Electrochemistry calculations for ion-air battery materials.
- **Software development:** parsers for simulation softwares I/O files. Automatic workflow for high-throughput simulation management.
- **Supervising and coaching:** 9 students internships. Python and Machine learning coach. **Technical validator** python.

Research Assistant — 2016 – 2018
Basel University — Basel (CH)

- Nccr-Marvel project & ChemSpaceLab: ab-initio materials design
- QMAT-x: a reference dataset for crystallographic machine learning
- Quantum Machine Learning for electronic transport properties
- Invited Research Fellow at The University of California (USA):
  Long research program of the Institute for Pure and Applied Mathematics:
  "Complex High-Dimensional Energy Landscapes" (whitepaper)

PhD Student — 2011 – 2016
Liège University - Nanomat — Liège (Be)

- FNRS-FRIA personal fellowship (Ph.D. Thesis)
- Theory and software development in ABINIT: temperature-dependent transport properties (Seebeck coefficient, electrical resistivity)
- Visiting Researcher at The University of Texas at Austin (TX, USA):
  Magnetic proximity effects at heavy metal-magnetic interfaces
- Spintronics, Spin-Caloritronics, Thermoelectrics, Piezoelectrics: Coupled thermal, magnetic and electronic excitations effect on nano-transport
- Spin-waves propagation in Permalloy
- Thermal excitations and dynamical stability of Calcium

Undergrad Student — 2005 – 2011
Bari University — Bari (IT)

- **Master Degree** Replica trick in a finite size spin glass (PDF).
  Internship: (INFN-IT) Random matrices
- **Bachelor Degree** Simulated evolution (PDF).
  Internship: (LIMPH-FR) Electronic structure with Monte Carlo methods.
  Erasmus project: Sorbonne University - Paris Nord/CNRS.
  Student union representative.
  Private after school classes

LANGUAGES

Italian (Mother)	●●●●●
English	●●●●●
French	●●●●●
Spanish	●●●○○
German	●●○○○
Dutch	●○○○○
Portuguese (Br.)	●○○○○

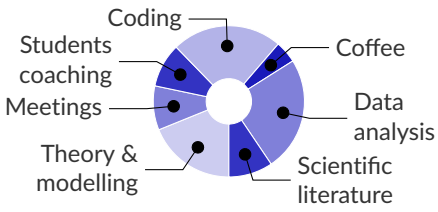
EDUCATION

- Ph.D. Science — 2015
  Liége University (Be)
- MS Theoretical Physics — 2010
  110/110 cum laude — Bari University (It)
- BS General Physics — 2008
  110/110 — Bari University (It)
- Liceo scientifico — 2005
  95/100 — Ruvo di Puglia (It)

PUBLICATIONS

Int. J. Hydrog **021**, 27612, 2021
Phys. Rev. B **102**, 155128, 2020
Phys. Rev. B **97**, 214417, 2018
Com. Phys. Comm. **205**, 106, 2016
Phys. Rev. Lett. **111**, 025503, 2013

ONE DAY AT WORK



LEISURES

Sports: Ultimate Frisbee, climbing
Dance: Lindy Hop
Outdoor activities
Language tandem