CV FRONT PAGE

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| Surname, first name: | Di Gennaro, Marco | | | | | | |
| Date of last update: | 04/2024 | | | | | | |
| e-mail address: | paola.dicaro@emeal.nttdata.com | | | | | | |
| External service provider information: | Date of birth: 01/12/1986 | | Nationality: Italian | | | | |
| Type of contract: | Employer: NTT Data   * Permanent (Check the appropriate) * Non-permanent * Freelancer:   Name of freelance company:  Atomistic Modelling | | | | Date of recruitment: At signature of S.C  Number of months working for the tenderer: 0 months  Comments: ……………………………  ………………………………………. | | |
| Current function: | Data Scientist | | | | Freelance Data Scientist – Project Manager | | |
| Profile for which external service provider is entered: | Database Architect | | | Date available: 01/05/2024 | | | |
| Highest relevant educational qualification: | Check the appropriate:   * Master degree or equivalent (≥4 years) * Bachelor degree * Secondary school   Number of (successful) years of study after secondary school: 9 | Certificate or diploma:  PhD Computational Physics  Institute: University of Liege (Be) | | | | | End date of secondary school:  (mm/yy): 06/05  Start date of higher studies:  (mm/yy): 09/05  End date of studies (mm/yy):  09/2010 |
| Languages:  (indicate level of skill: from 1=basic to 5=excellent) | English:  French:  German:  Other(s): Italian  Spanish  Dutch  Portuguese | Spoken  5  5  2  5  3  1  1 | | | | | Written  5  5  2  5  3  1  1 |
| Professional experience | Date IT career started: 03/2011 | | | | | Number of years/months of experience (apart from the studies): 13 years/156 months | |
| Specific expertise(s) (with number of months experience for each) | Research and Development (R&D) = 156 months  Theoretical Physics = 156 months  Quantum Chemistry = 156 months  Computer Science = 156 months  Data Visualization = 156 months  High Performance Computing = 156 months  Algorithms = 120 months  Multiscale Material Simulation = 120 months  Big Data & Data Science = 120 months  Machine Learning = 96 months  Statistical analysis = 60 months  Numerical Methods = 156 months  Software Development = 156 months  Time series analysis = 12 months  Cloud Computing = 12 months  Density Functional Theory (DFT) = 96 months  Molecular Dynamics (MD) = 72 months  Materials Informatics = 60 months  Complex Systems Modelling = 60 months  Quantum Computing = 24 months  Monte Carlo Simulations = 12 months  Coaching = 24 months  Scientific Writing = 156 months  Public Speaking = 60 months | | | | | | |
| Standard(s) or certificate(s) |  | | | | | | |
| Proposed level | 9 | | | | | | |

CV Summary

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| With over 15 years in materials science and machine learning, my career is centred around innovative projects in batteries, fuel cells, spintronic materials, and gas adsorption processes. I leverage data science, materials simulation and quantum computing to address complex challenges in materials science, enhancing our capabilities in application driven, computational materials design.  As the founder of Atomistic Modelling, I focus on understanding the properties and applications of materials for battery electrolytes, improving photo-catalysts, and advancing the use of nanomaterials. These endeavours are part of my larger goal: to contribute to decarbonization through material innovation.  My dream is to discover and develop materials that will play a crucial role in reducing carbon emissions. To achieve this, I collaborate with researchers, industry partners, and clients who share this vision of a more sustainable future. I am always eager to engage in discussions, learn from others, and explore new ideas in this rapidly evolving field, with the hope of making a significant impact on our planet's and people health and security. |

CV training page

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| CV training page number for this CV: | 1 |

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| TRAINING | | | | |
|  | Training name: | Company/institute organising the training: | Date(s) training followed: | Exams or certificates: |
|  | Introduction to MongoDB | Coursera | 2020 | Certificate |
|  | Linux admin | Cevora | 2019 | Certificate |
|  | Introduction to SQL | Evoliris | 2018 | Certificate |
|  | AWS Cloud Practitioner | AWS | 2024 | Exam |
|  | Toefl (test of English as a foreign language) | Educational Testing Service (ETS) | 2010 | Exam |
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CV software expertise page

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| CV software expertise page number for this CV: |  |

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| Software expertise | | | | |
|  | Tool (when possible precise manufacturer, product name and version(s)) | Competence (rating: 1 -5) | Duration (in months) | Description (reference to relevant entries under “professional experience” is mandatory) |
| 1 | Bash | 5 | 156 | Software Development: 1, 2, 4, 5, 6, 7 |
| 2 | HPC | 5 | 156 | High Performance Computing: 1, 2, 4, 5, 6, 7 |
| 3 | Latex | 5 | 156 | Advanced typesetting: 1, 2, 4, 5, 6, 7 |
| 4 | Linux | 5 | 156 | System administration: 1, 2, 4, 5, 6, 7 |
| 5 | Microsoft Office | 5 | 156 | Office Suite: 1, 2, 3, 4, 5, 6, 7 |
| 6 | Numpy, Scipy, Pandas | 5 | 156 | python libraries for data science: 1, 2, 4, 5, 6, 7 |
| 7 | Python | 5 | 120 | Software Development: 1, 2, 4, 5, 6, 7 |
| 8 | Abinit | 5 | 60 | DFT Calculations: 1, 2, 4, 5, 6, 7 |
| 9 | Scikitlearn | 5 | 60 | Machine Learning: 1, 2, 4, 5 |
| 10 | Github | 4 | 60 | System Control, CI/CD: 1, 2, 4, 5, 6, 7 |
| 11 | Gromacs | 4 | 36 | MD Calculations: 1, 2, 4, 5 |
| 12 | Lammps | 4 | 36 | MD Calculations: 1, 2, 4, 5 |
| 13 | Materials Project | 4 | 36 | Materials Informatics Workflow Engine: 1, 2, 4 |
| 14 | AWS | 4 | 24 | Cloud Computing: 1, 2 |
| 15 | Pytorch | 4 | 24 | Machine Learning: 1, 2, 4, 5 |
| 16 | Turbomole | 4 | 24 | DFT Calculations: 1, 2 |
| 17 | Wordpress | 4 | 24 | Website design: 1 |
| 18 | C++ | 3 | 24 | Software Development: 1, 2, 4, 5, 6 |
| 19 | MongoDB | 3 | 24 | Non-Relational Database Management: 1, 2 |
| 20 | SQL | 3 | 24 | Relational Database Management: 1, 2 |
| 21 | Aiida | 3 | 12 | Materials Informatics Workflow Engine: 1, 2, 4, 5 |
| 22 | GCP | 3 | 12 | Cloud Computing: 1, 2 |
| 23 | Keras | 3 | 12 | Machine Learning: 1, 2, 4 |
| 24 | Qiskit | 3 | 12 | Quantum computing library: 1, 2 |
| 25 | Quantum Espresso | 3 | 12 | DFT Calculations: 1, 2, 4, 5, 6**, 7** |

CV professional experience page

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| CV experience page number for this CV: | 1 |

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| PROJECT EXPERIENCE | |
| Project name: | Materials informatics for automotive applications |
| Company (employer): | Atomistic Modelling |
| Dates (start-end):  Effective number of months achieved: | 03/2023 – 02/2024  12 months |
| Client (customer): | Toyota Motor Europe |
| Project size: | Medium: 6 people involved, 140k euro budget |
| Project description:   * Batteries:   + 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:   + 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 * Post DFT methods to design semiconductor for water photo-catalysis | |
| External service provider’s roles & responsibilities in the project:  Role: Founder & Freelance consultant  • 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 | |
| Technologies and methodologies used by the external service provider in the project:  Bash, HPC, Latex, Linux, Microsoft Office, Numpy, Scipy, Pandas, Python, Abinit, Scikitlearn, Github, Gromacs, Lammps, Materials Project, AWS, Pytorch, Turbomole, Wordpress, MongoDB | |

CV professional experience page

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| CV experience page number for this CV: | 2 |

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| PROJECT EXPERIENCE | |
| Project name: | Machine Learning for Automotive |
| Company (employer): | Toyota Motor Europe |
| Dates (start-end):  Effective number of months achieved: | 06/2018 – 02/2023  57 months |
| Client (customer): | Toyota Motor Europe |
| Project size: | Large: > 10 people involved |
| Project description:   * Fuel cells   + Application-driven material design for thermodynamical H2 storage   + Developed a pipeline to manage vast amount of simulations   + Computational pipeline to simulate ∼150k Metal Organic Frameworks   + Feature Selection & Genetic Algorithm for H2 adsorption into crystals * Batteries:   + Electrothermal simulations of liquid electrolysers for Li-O2 batteries * Nanomaterials: Calculated stress-strain resistance of carbon nano tubes and enhanced resistance with cross-functional linking for high pressure H2 storage * Gas exhaust catalysis: Clustering model to translate over 1M chemical hydrocarbon reactions into simplified (5-10), efficient model for human analysis * Lubricants: Explained tribological macroscopic effects from molecular interactions, Benchmark of several physics-inspired ML models, Feature Selection * Quantum computing algorithms to improve classical materials simulations for photo-catalysis * Internal training: delivered series of seminars on python and machine learning | |
| External service provider’s roles & responsibilities in the project:  Role: Machine Learning Scientist  • 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 | |
| Technologies and methodologies used by the external service provider in the project:  Bash, HPC, Latex, Linux, Microsoft Office, Numpy, Scipy, Pandas, Python, Abinit, Scikitlearn, Github, Gromacs, Lammps, Materials Project, AWS, Pytorch, Turbomole, C++, MongoDB, SQL, Aiida, GCP, Keras, Qiskit, Quantum Espresso | |

CV professional experience page

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| CV experience page number for this CV: | 3 |

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| PROJECT EXPERIENCE | |
| Project name: | Bicification |
| Company (employer): | Pin Bike, Corato (It) |
| Dates (start-end):  Effective number of months achieved: | 01/2021 – 06/2021  6 months |
| Client (customer): | Pin Bike |
| Project size: | Medium: 10 people, 300000 eur |
| Project description:  Pin Bike remunerates people to use their bike instead of their car in urban displacements. | |
| External service provider’s roles & responsibilities in the project:  Role: Freelance Project Manager EU Projects  • Bicification EIT urban mobility project: pitch competition, budget negotiations (∼e300K), partnership agreements and recruitment. | |
| Technologies and methodologies used by the external service provider in the project:  Microsoft Office, Wordpress | |

CV professional experience page

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| CV experience page number for this CV: | 4 |

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| PROJECT EXPERIENCE | |
| Project name: | Complex High-Dimensional Energy Landscapes |
| Company (employer): | IPAM – UCLA, Los Angeles (USA) |
| Dates (start-end):  Effective number of months achieved: | 09/2017 – 12/2020  40 months |
| Client (customer): | IPAM – UCLA, Los Angeles (USA) |
| Project size: | Large (~100 people) |
| Project description:  Recent advances in computational resources and the development of high-throughput frameworks enable the efficient sampling of complicated multivariate functions. This includes energy and electronic property landscapes of inorganic, organic, biomolecular, and hybrid materials and functional nanostructures. Combined with the recent focus on data science and the materials genome initiative, this leads to a rapidly growing need for numerical methods and a fundamental mathematical understanding of efficient sampling approaches, optimization techniques, hierarchical surrogate models and coarse graining techniques, and methods for uncertainty quantification.  The complexity of these energy and property landscapes originates from their simultaneous dependence on discrete degrees of freedom (e.g. number of atoms and species types) and continuous ones (e.g. position of atoms). The complexity is further exacerbated by the presence of divergences (e.g. when atoms approach one another and at critical transition points) and non-trivial emergent phenomena that are due to collective interactions. Moreover, dynamical behavior governed by complex landscapes involves a rich hierarchy of timescales and is characterized by rare events that often are key to understanding function of the molecular structures under investigation. This complexity provides an ideal test bed for novel mathematical methods that characterize these functions and provide a description as well as optimal numerical methods.  This program will bring together researchers from pure and applied mathematics, computer science, materials science, chemistry, physics, and biomolecular science to advance the understanding of simulation, stochastic sampling and optimization methods for multidimensional energy landscapes and to develop a common language. | |
| External service provider’s roles & responsibilities in the project:  Role: Invited Fellow  • Long research program: Complex High-Dimensional Energy Landscapes  • Engaged in applied mathematics & multi-disciplinary team work | |
| Technologies and methodologies used by the external service provider in the project:  Bash, HPC, Linux, Numpy, Scipy, Pandas, Python, Scikitlearn, Gromacs, Lammps, Materials Project , Keras | |

CV professional experience page

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| CV experience page number for this CV: | 5 |

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| PROJECT EXPERIENCE | |
| Project name: | PostDoc in Quantum Machine Learning |
| Company (employer): | University of Basel, Basel (CH) |
| Dates (start-end):  Effective number of months achieved: | 08/2016 – 05/2018  22 months |
| Client (customer): | University of Basel, Basel (CH) |
| Project size: | Medium ~10 people |
| Project description:   * 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 | |
| External service provider’s roles & responsibilities in the project:  Role: Research Assistant  • Integrated theoretical chemistry and machine learning  • Managed multiple projects with a focus on strategic prioritisation  • Organising Committee: The 2017 Basel Postdoctoral Network Retreat | |
| Technologies and methodologies used by the external service provider in the project:  Bash, HPC, Latex, Linux, Microsoft Office, Numpy, Scipy, Pandas, Python, Abinit, Scikitlearn, Github, Gromacs, Lammps, Materials Project, AWS, SQL, Aiida, Quantum Espresso | |

CV professional experience page

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| CV experience page number for this CV: | | 6 |
| PROJECT EXPERIENCE | | |
| Project name: | Scientific Collaborator | |
| Company (employer): | Liège University – Nanomat, Liege (Be) | |
| Dates (start-end):  Effective number of months achieved: | 10/2011 – 07/2016  54 months | |
| Client (customer): | Liège University – Nanomat, Liege (Be) | |
| Project size: | 5 people | |
| Project description:  Study of temperature dependence of spin-wave propagation stiffness | | |
| External service provider’s roles & responsibilities in the project:  Role: Scientific Collaborator  • Research in computational solid-state physics: modelling of complex phenomena | | |
| Technologies and methodologies used by the external service provider in the project:  Bash, HPC, Latex, Linux, Numpy, Scipy, Pandas, Python, Abinit, Github | | |

CV professional experience page

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| CV experience page number for this CV: | | 7 |
| PROJECT EXPERIENCE | | |
| Project name: | Spin-Caloritronics materials | |
| Company (employer): | F.N.R.S. - Liège University – Nanomat, Liege (Be) | |
| Dates (start-end):  Effective number of months achieved: | 03/2011 – 09/2015  54 months | |
| Client (customer): | F.N.R.S. - Liège University – Nanomat, Liege (Be) | |
| Project size: | 5 people | |
| Project description:  Spin-Caloritronics materials  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   * 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   * Explained unusual crystallographic phase transition of Calcium via DFT   Visiting Student at the university of Texas at Austin | | |
| External service provider’s roles & responsibilities in the project:  Role: PhD Student (FRIA-FNRS personal grant)  • Project management: running research grant of e10k 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) | | |
| Technologies and methodologies used by the external service provider in the project:  Bash, HPC, Latex, Linux, Numpy, Scipy, Pandas, Python, Abinit, Github, Materials Project, C++, Quantum Espresso | | |