europass

Pierluigi Mario Strazzanti

Date of birth: [redacted] | **Place of birth:** [redacted] | **Nationality:** [redacted] |

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WORK EXPERIENCE

CNR-IMM SEDE CATANIA – CATANIA, ITALY

Address VIII strada, 5 (Zona Industriale), 95121, Catania, Italy

RESEARCH FELLOW – 01/07/2024 – 30/06/2025

Projects:
-Innovation Grant between Centro Nazionale di Ricerca in High Performance Computing, Big Data e Quantum Computing PNRR - Spoke 7 Materials & Molecular Sciences and ENI S.p.A.
Project title: Accelerating the pace of the energy transition through simulation-guided discovery of advanced green materials.
Scope: Study of CO2 Adsorption on Amorphous Carbon Materials Using Molecular Dynamics and Machine Learning.

Experience in using high-performance computing resources on the Leonardo partition of the CINECA supercomputer. Proficient in atomic-scale simulations using ASE and LAMMPS for molecular dynamics. Trained in developing machine learning-based interatomic potentials with frameworks such as NequIP, ALLEGRO, and MACE.

-Project: Industrial Research Project between CNR-IMM and SCREEN Semiconductor Solutions Co., Ltd. Japan
Scope: Innovative green solvents by Artificial Intelligence and Molecular Dynamics.

EDUCATION AND TRAINING

08/04/2025 – 11/04/2025 Casalecchio di Reno, Italy

INTRODUCTION TO PYTHON, CINECA TRAINING COURSE CINECA

Introductory course focused on the use of Python in scientific applications and data science.

Website https://www.cineca.it/it

06/01/2025 – 17/01/2025 AMSTERDAM, Netherlands

MOLSIM2025 2-WEEK FLAGSHIP SCHOOL CECAM-UNIVERSITY OF AMSTERDAM

MolSim-2025 is a two-week school which deals with Molecular Dynamics and Monte Carlo simulations applied to material science.

Website https://www.cecam.org/workshop-details/molsim-2025-1335

Catania, Italy

MASTER DEGREE IN MATERIALS CHEMISTRY University of Catania - Chemistry department

Website https://www.dsc.unict.it/ | **Thesis** Organic electronics: the role of P3HT and PEDOT:PSS

PRE-DEGREE TRAINING INTERNSHIP LAMSUN-University of Catania

Experimental internship at the LAMSUN Laboratory (Laboratory of Molecular Surface and Nanotechnologies), University of Catania, focused on the physical-chemistry of surfaces. The work was conducted in the field of organic electronics, with hands-on experience in processing and analyzing materials such as P3HT, PEDOT:PSS, and single-

walled carbon nanotubes (SWCNTs). Characterization techniques included Atomic Force Microscopy (AFM) and Linear Sweep Voltammetry (LSV).

Catania, Italy
BACHELOR'S DEGREE IN CHEMISTRY University of CATANIA

Website https://www.dsc.unict.it/ | **Thesis** Nanoconfinement of Laminin: a free energy study

LANGUAGE SKILLS

Mother tongue(s): **ITALIAN**

Other language(s):

	UNDERSTANDING		SPEAKING		WRITING
	Listening	Reading	Spoken production	Spoken interaction	
ENGLISH	B2	B2	B2	B2	B2

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

SKILLS

Molecular dynamics | Machine Learnings | python programming | Experience in HPC environments and working with SLURM scheduler | Microsoft Office | Windows | Origin (data analysis) | Social Network | EXPERIMENTAL CHEMISTRY | data science | ubuntu

CONFERENCES AND SEMINARS

02/06/2025 – 05/06/2025 Karlsruhe, Germany
CECAM Workshop "Virtual Materials Design: AI, Simulation, and Workflows" at Karlsruhe Institute of Technology

Participated in a scientific event on ML techniques applied to materials science and presented my poster "Classical and ML FFs for carbon dioxide".

Link https://www.cecam.org/workshop-details/virtual-materials-design-ai-simulation-and-workflows-1398

06/01/2025 – 17/01/2025 Amsterdam (Netherlands)
Molsim-2025

Author of the poster titled "Classical and machine learning force fields for carbon dioxide" with authors: P. Strazzanti, I. Vacante, G. Calogero, D. Ricciarelli, I. Deretzis, A. La Magna, G. Fisicaro

Link https://www.cecam.org/workshop-details/molsim-2025-1335

08/01/2025 – 10/01/2025 Trieste (Italy)
22nd International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods | (SMR 4050)

Co-author of the poster titled "Structural models of amorphous C-based materials from machine learning interatomic potentials", presented by G. Fisicaro with authors: I. Vacante, P. Strazzanti, G. Calogero, D. Ricciarelli, I. Deretzis, A. La Magna, G. Fisicaro

Link https://indico.ictp.it/event/10815/overview

17/09/2024 – 20/09/2024 Rome (Italy)
ICSC Annual Meeting 2024

Participation in the Annual Meeting of the National Research Center in HPC, Big Data, and Quantum Computing, which provided an opportunity for discussion and sharing of activities carried out and future objectives for the entire large ICSC community.

Link https://agenda.supercomputing-icsc.it/event/2/

REPORT & DELIVERABLES

Report Milestone 8 Work package 1.1 - Innovation Grant ENI

Report on the activities carried out for Milestone 8, work package 1.1, by the research group of CNR IMM Catania section within the framework of the Innovation Grant ENI HPC Spoke 7 project. The report documents the progress related to the training of machine learning interatomic potentials (NequIP) and the determination of a workflow to train, verify the accuracy, and validate the potential, with relevant examples using a dataset found in the literature and one produced by CNR IOM. For confidentiality reasons, the report is not publicly accessible.

Report Milestone 9, Work package 1.3 - Innovation Grant ENI

Report on the activities carried out for Milestone 9, work package 1.3, by the research group of CNR IMM Catania section within the framework of the Innovation Grant ENI HPC Spoke 7 project. The report contains the description of the testing procedure for NequIP and Allegro interatomic potentials to evaluate the computational cost for the same level of accuracy in the selection of hyperparameters. Furthermore, the impact of adding corrections related to dispersion forces was evaluated in the aforementioned potentials and in MACE, trained on the dataset produced by CNR IOM. For confidentiality reasons, the report is not publicly accessible.

Deliverable 3.1 Screen Japan

Contributed to the deliverable for Milestone 3.1 of the SCREEN project. Due to confidentiality agreements, the deliverable is not publicly accessible.

COMMUNICATION AND INTERPERSONAL SKILLS

Team working skills

Strong teamwork skills developed through bachelor’s and master’s studies, further strengthened during my research grant at IMM, and enriched by years of volunteering, sports activities, and playing a musical instrument. My communication and interpersonal abilities have also been enhanced through extensive private tutoring in general and organic chemistry.