

# Paolo De Angelis

## Curriculum Vitae

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Portfolio [↗](#)



**Date of birth:** 11/11/1993

**Sex:** Male; **Nationality:** Italian

## Research Experience

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|-----------|---|
| 2023–Now  | <b>PostDoc in Energetics, Politecnico di Torino, Italy.</b><br>SUPERVISOR: Prof. Eliodoro Chiavazzo<br>TOPIC: Atomistic simulation of electrodes of electrochemical storage batteries.  |
| 2022–2023 | <b>Research fellowship in Energetics, Politecnico di Torino, Italy.</b><br>SUPERVISOR: Prof. Eliodoro Chiavazzo<br>TOPIC: Revealing structure-properties relationship of the battery materials using machine learning (ML) informed by ab-initio density functional theory (DFT) and phase-field modelling (PFM). |
| 2020–2020 | <b>Visiting PhD Student, University of Illinois at Chicago, USA.</b><br>SUPERVISOR: Prof. Farzad Mashayek<br>TOPIC: Atomistic modeling of degradation phenomena at battery electrodes.  |

## Education

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|-----------|---|---------------------------|
| 2018–2022 | <b>PhD in Energetics, Politecnico di Torino, Italy.</b><br>SUPERVISOR: Prof. Pietro Asinari, Prof. Eliodoro Chiavazzo, Prof. Daniele Marchisio<br>THESIS: Reactive and Non-Reactive Interface Modelling for Energy Materials.<br>MARK: 110L/110 | 3rd cycle degree - PhD    |
| 2015–2017 | <b>MSc in Mechanical Engineering, Politecnico di Torino, Italy.</b><br>LANGUAGE: English<br>THESIS: Simulation of the ensemble and cycle-resolved combustion processes in a NG-H2 engine.<br>MARK: 110/110                                      | 2nd cycle degree - Master |
- Related document: *Attachment–University transcript*

	Related document: <i>Attachment–University transcript</i>	
2012–2015	<b>BSc in Mechanical Engineering, Politecnico di Torino, Italy.</b>	1st cycle degree - Bachelor
	LANGUAGE: Italian THESIS: Quaternion application to 3D roto-translation on simulative environment. MARK: 107/110	
	Related document: <i>Attachment–University transcript</i>	
2007–2012	<b>Scientific diploma, Liceo scientifico of San Benedetto del Tronto, Italy.</b>	Italian secondary school diploma
	ISTITUTE NAME: Liceo scientifico – B.Rosetti GRADE: 84/100	

## Teaching Experience

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2021–Now	<b>Applicazioni energetiche dei materiali</b> for MSc students in Energetics engineering LANGUAGE: Italian ISTITUTE NAME: Politecnico di Torino, Italy
2021–Now	<b>Energy storage</b> for MSc students in Energetics engineering LANGUAGE: English ISTITUTE NAME: Politecnico di Torino, Italy

## Work experience

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2017	<b>MCA Engineering</b> Student internship where I start the work that I will continue in the thesis. I worked in parallel with the GasOn project, that is a European project with many automobile manufacturers drive by Renault, where my role was to study of the model numerical stability and efficiency, with focus on the combustion models.
2014–2015	<b>Part-Time Collaborations – Politecnico di Torino</b> During the second semester I worked for 100 hours to help professors during lessons of Calculus I & II, and also the students after lesson.
2009–2012	<b>Real Due s.a.s</b> I Worked 3 months during summer as apprentice in a small job shop specialized in building and repairing trailers for trucks and the assembly of ANTEO tail-lifts. During which I helped to produce intermediate material and I drew some simple components to send to external suppliers, thus I have learned how use manual drilling machine, MIG welder and band-saw, and to carry out other elementary task (e.g. bearing mounting and assembly and electrical motor maintenance ).

## Conference Contributions

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- 2022 **2022 MRS Spring Meeting**  
 ORGANIZER: MRS – Materials Research Society  
 VENUE: Hawai'i Convention Center, Honolulu, USA.  
 CONTRIBUTION: Speech on the topic “*A Consistent and Interactive Protocol for Generating an Atomistically Resolved Solid Electrolyte Interphase (SEI) Passivating Layer in Li-Ion Batteries*”.
- 2020 **APS March Meeting 2020**  
 ORGANIZER: APS – American Physical Society  
 VENUE: Denver, USA.  
 CONTRIBUTION: Speech on the topic “*Exploring the free energy landscape to predict surfactant adsorption isotherm at nanoparticle-water interface*”.
- PRiME 2020**  
 ORGANIZER: ECS – Electrochemical Society  
 VENUE: Online, WWW.  
 CONTRIBUTION: Speech on the topic “*Combined Multi-Physics and Machine Learning Approach to Forecast SEI Decomposition in LIBs*”.
- 2019 **Mainz Materials Simulation Days 2019**  
 ORGANIZER: CECAM – Centre Européen de Calcul Atomique et Moléculaire  
 VENUE: Max Planck Institute for Polymer Research, Mainz, Germany.  
 CONTRIBUTION: Poster presentation with the title “*Free Energy Landscape by Steered Molecular Dynamics to predict surfactant adsorption isotherm*”.

## Publications

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- 2022 Roberta Cappabianca, **De Angelis, Paolo**, Annalisa Cardellini, Eliodoro Chiavazzo, and Pietro Asinari. "Assembling Biocompatible Polymers on Gold Nanoparticles: Toward a Rational Design of Particle Shape by Molecular Dynamics." *ACS Omega* 7, no. 46 (2022): 42292-42303 doi:[10.1021/acsomega.2c05218](https://doi.org/10.1021/acsomega.2c05218)
- 2021 **De Angelis, Paolo**, Marta Tuninetti, Luca Bergamasco, Luca Calianno, Pietro Asinari, Francesco Laio, and Matteo Fasano. "Data-driven appraisal of renewable energy potentials for sustainable freshwater production in Africa." *Renewable and Sustainable Energy Reviews* 149, (2021): 111414. doi:[10.1016/j.rser.2021.111414](https://doi.org/10.1016/j.rser.2021.111414)
- 2020 **De Angelis, Paolo**, Vitaliy Yurkiv, Pietro Asinari, and Farzad Mashayek. "Combined Multi-Physics and Machine Learning Approach to Forecast SEI Decomposition in LIBs." *ECS Meeting Abstracts* no. 4, p. 777., IOP Publishing, (2021): 111414. doi:[10.1149/MA2020-024777mtgabs](https://doi.org/10.1149/MA2020-024777mtgabs)
- 2019 **De Angelis, Paolo**, Annalisa Cardellini, and Pietro Asinari. "Exploring the Free Energy Landscape To Predict the Surfactant Adsorption Isotherm at the Nanoparticle–Water Interface." *ACS central science* 5, no. 11 (2019): 1804-1812. doi:[10.1021/acscentsci.9b00773](https://doi.org/10.1021/acscentsci.9b00773)

## Personal Skills

Mother tongue **Italian**

Other language **English – Independent user**

Understanding		Speaking		Writing
Listening	Reading	Spoken interaction	Spoken production	
B1 (4.5)	C1 (6.5)	B2 (5)	B2 (5)	B2 (5.5)
B2 (IELTS 5.5)*				

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

☞ Common European Framework of Reference for Languages (CEFR)

☞ IELTS Band Score vs CEFR Levels

\*This mark is refer to the IELTS exam made in 13 December 2014, then thank the master and thesis work I quite improve my language skills

Digital competence

### SELF-ASSESSMENT

Information processing	Communication	Content creation	Safety	Problem solving
Proficient user	Proficient user	Proficient user	Independent user	Independent user

☞ CEFR Levels Digital competences - Self-assessment grid

Operating system

WINDOWS: Quite high level of knowledge, Version used 10, 8.1, 8, 7, XP, 2000, 98, 95.

LINUX: Medium-high level of knowledge, Distribution use: Ubuntu (v: 18.04, 19.04, 12.04, 11.04, 9.04), Mint (v: 9, 8), openSUSE (v: 42.2, 12.2).

CAD programs

SOLIDWORKS: I have learned to use this CAD software in two courses of bachelor degree that is “Disegno tecnico industriale”(EN:Engineering drawing) and “Elementi di costruzione e disegno di macchine”(EN:Fundamentals of machine design and drawing). And I used it also in other courses as drawing tool for some project.

AUTOCAD: I used it for 2D drawing of plant layout of a medium size industry as project for the course “Impianti industriali e sicurezza sul lavoro”(EN:Industrial plants and safety), thus I attended a brief course to learn the bases of software and then I increased the knowledge by my own.

Programming languages

C: I know the medium level elements of programming in C thanks the course “Informatica”(EN:Computer sciences) during the university’s first year.

PYTHON: Self taught knowledge achieved by trying to find a Open-Source alternative to Matlab, e.g. using the scientific library NumPy of the project <http://ipython.org>.

MATLAB: I used it for first time during thesis for developing scripts to manipulate the stiffness and damping matrix of a FEM model using quaternion operator. Then I attended the course of “Numerical modelling” where I have learned the 3 main numerical PDE’s solver techniques: FDM, FEM and FVM. Hence during the applied lecture I developed some scripts to solve thermal and elastic (1D and 2D) problems.

SE solvers

QUANTUM ESPRESSO: Used during the Ph.D. course “Introduction to DFT” by Prof. Giancarlo Cicero where we studied the properties of bulk and surface of pure silicon.

SCM BAND: Atomic-orbital based DFT engine extensively used during my PhD to produce the training set for the ReaxFF force field parameterization for the LiF crystal.

<i>ODE solvers</i>	GROMACS: It is a Molecular Dynamics (MD) code used during the first Ph.D. year. Namely for Non-Equilibrium MD and Free Energy studies.
	LAMMPS: Molecular Dynamics (MD) code used during the my Ph.D. years. Namely for Reactive MD (with ReaxFF force field) and Free Energy studies.
<i>PDE solvers</i>	CONVERGE: Used during the internships(3 months) and thesis (6 months) to develop a CFD model of a methane engine, with focus on combustion, mesh refinement, and RANS turbulence model.
	COMSOL MULTIPHYSICS: Used during the course “Numerical design of thermal systems” for the applied lecture where we designed a furnace of the waste-to-energy plan and a thermal energy storage.
	OPENFOAM: Self taught knowledge, used to have a deep understand of Finite Volume method and numerical methods following the exercise and problems of the book “The Finite Volume Method in Computational Fluid Dynamics” - Moukalled, Mangani, Darwish.
<i>Office suite</i>	MICROSOFT OFFICE: High knowledge of Word and Powerpoint, Medium-High of Excel and Basis knowledge of Access and Project. I currently use the 2016 version(2013 for Project) but I used also older version like Office 2003 and 97.
	LIBREOFFICE: Open Source alternatives of Microsoft Office suite, used since I worked also in Linux environment. I actually use the 5.3 version.
	L <sup>A</sup> T <sub>E</sub> X: I use it since the High School, when I learned it during math lesson and then I improved the knowledge by my own. Indeed I used it to write technical report, the thesis and this CV.
<i>Other</i>	ARDUINO: Studied for the exam “Hydraulic and thermal machines testing” where we developed simple DAQ using it, by changing the frequency of its internal clocks. Then I continue to use as hobby to build simple instruments or to acquire data.

**Attachment–University transcript****Master's degree: Mechanical Engineering**

	<b>Exam</b>	<b>Grade</b>	<b>Date</b>	<b>ECTS</b>
1	Thermal and hydraulic machines	26/30	16/02/2016	10
2	Business Economics and Organization	30L/30	17/06/2016	8
3	Advanced engineering thermodynamics/Numerical modelling	27/30	05/07/2016	10
4	Machine design	27/30	07/09/2016	8
5	Integrated Manufacturing Systems	23/30	22/09/2016	6
6	Vibration mechanics	28/30	23/02/2017	8
7	Numerical design of thermal systems	30L/30	01/03/2017	8
8	Dynamic design of machines	29/30	19/06/2017	10
9	Mechanical system dynamics	30L/30	19/06/2017	6
10	Stage (Internships)	passed	22/06/2017	12
11	Hydraulic and thermal machines testing	30/30	11/09/2017	10
12	Materials for mechanical industries	26/30	15/09/2017	6

**Master's degree: Mechanical Engineering**

	<b>Exam</b>	<b>Grade</b>	<b>Date</b>	<b>ECTS</b>
1	Analisi matematica I	30/30	28/01/2013	10
2	Chimica	20/30	21/02/2013	8
3	Storia dell'energia	28/30	01/07/2013	6
4	Informatica	28/30	05/07/2013	8
5	Fisica I	27/30	08/07/2013	10
6	Geometria	24/30	18/09/2013	10
7	Disegno tecnico industriale	27/30	31/01/2014	6
8	Analisi matematica II	30/30	03/02/2014	6
9	Fisica II	27/30	13/02/2014	6
10	Fondamenti di meccanica strutturale	26/30	20/02/2014	8
11	Statistica sperimentale e misure meccaniche	30L/30	07/07/2014	6
12	Scienza e tecnologia dei materiali/Tecnologia dei materiali metallici	28/30	17/07/2014	10
13	Termodinamica applicata e trasmissione del calore	27/30	02/09/2014	8
14	Meccanica applicata alle macchine	30/30	10/09/2014	10
15	Lingua inglese I livello	passed	13/12/2014	3
16	Elementi di costruzione e disegno di macchine	28/30	26/01/2015	12
17	Tecnologia meccanica	26/30	04/02/2015	8
18	Elettrotecnica/Macchine elettriche	27/30	16/02/2015	10
19	Impianti industriali e sicurezza sul lavoro	26/30	10/07/2015	10
20	Fondamenti di macchine e di oleodinamica	30/30	15/07/2015	10
21	Meccanica dei fluidi	28/30	07/09/2015	6
22	Matematica applicata	30L/30	15/09/2015	6
23	Prova finale	passed	09/12/2015	3