PERSONAL INFORMATION

Angelo Damone

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Linkedin, Research Gate, Google Scholar

Skype angelo.magnetar

Gender Male | Date of birth 21 May 1989 | Nationality Italian

EDUCATION AND TRAINING

2014 – 2017

Ph.D. in Mechanical and Industrial Engineering

University of Brescia, Brescia, Italy

Main Subjects Ph.D. : Molecular Dynamics, Numerical Simulation

Thesis Title : Hybrid Atomistic-Continuum Modeling of Liquid-Liquid Interfaces by Molecular Dynamics

2011 – 2013

Master's Degree in Chemistry

University of Bari, Bari, Italy

Main Subjects Internship : Molecular Dynamics, Computational Chemistry

Thesis Title : Molecular Dynamics of metals applied to nuclear fusion technology

2008 – 2011

Bachelor's Degree in Chemistry

University of Bari, Bari, Italy

Main Subjects Internship : Organic Chemistry

Thesis Title : Multi-Walled Carbon Nanotubes Surface Functionalization with Dioxyranes

RESEARCH EXPERIENCE

Oct. 2019 – Present

Post-Doctoral Fellowship

French Institute of Petroleum - Energie Nouvelles (IFPEN),
1-4 Avenue du Bois Préau, 92852 Rueil-Malmaison, France

– Calculation of Transport Properties through Dissipative Particle Dynamics (DPD) applied to electrolyte solutions.

Jan. 2018 – Sep. 2019

Post-Doctoral Fellowship

Technische Universität Kaiserslautern,
Erwin-Schrödinger-Straße 44, 67653 Kaiserslautern, Germany

– Developing of transferable Force-Field for poly(oxymethylene) dimethyl ethers using Quantum-Mechanical calculation through Density Functional Theory (DFT).
– Molecular modelling of radicals applied to Overhauser Dynamic Nuclear Polarization (DNP) to study the polarization transfer and the coupling mechanism.
– Study of Maxwell-Stephan and Fickian diffusion coefficient using Non-Equilibrium Molecular Dynamics, PC-SAFT and Density Gradient Theory (DGT).
– Study of salting-out effect on the Lower Critical Solution Temperature (LCST) of the poly(N-isopropyl-acrylamide) using Molecular Dynamics.
– Hydrogen-Bond investigation on propanol oxydation reaction with trimethyl-N-oxyde through Molecular Dynamics simulation.

Sep. 2016 – Dec. 2016

Ph.D. Fellowship Abroad

Massachusetts Institute of Technology
77 Massachusetts Ave, Cambridge, MA 02139, U.S.A.

- Modelling of liquid-liquid interface by Molecular Dynamics simulation for Lennard-Jones and real liquids to study the slip length dependency from the shear rate.
- Hybrid-Atomistic Continuum modelling approach for the derivation of the pressure drop through the liquid-liquid interface inside nano-channels and applied shear rate.

Nov. 2014 – Dec. 2017

Ph.D. Research Activities

University of Brescia,
Via Branze 38, 25133 Brescia, Italy

- Modelling of liquid-liquid interface by Molecular Dynamics simulation for Lennard-Jones and real liquids to study the slip length dependency from the shear rate.
- Hybrid-Atomistic Continuum modelling approach for the derivation of the pressure drop through the liquid-liquid interface inside nano-channels and applied shear rate.
- Determination of transport properties such as shear viscosity and thermal conductivity for water-triethylamine liquid mixtures using Molecular Dynamics.

Sep. 2014 – Nov. 2014

Term-Contract Coworker

University of Bari,
Via Edoardo Orabona 4, 70125 Bari, Italy

- Developing of an atomistic model of Neutral Beam Injectors (NBI) for nuclear fusion technology using a native fortran code for the simulations of Solid-Gas interaction.
- Theoretical determination of Molybdenum-Caesium interaction using Density Functional Theory (DFT), Coupled-Cluster (CC) and Møller-Plesset Perturbation Theory (MP2).

Apr. 2013 – May 2013

Master Internship - Visiting Master Student

Consorzio RFX,
Corso Stati Uniti 4, 35127 Padua, Italy

- Developing of an atomistic model of Neutral Beam Injectors (NBI) for nuclear fusion technology using a native fortran code for the simulations of Solid-Gas interaction.
- Theoretical determination of Molybdenum-Caesium interaction using Density Functional Theory (DFT), Coupled-Cluster (CC) and Møller-Plesset Perturbation Theory (MP2).

Dec. 2012 – Dec. 2013

Master Internship

University of Bari,
Via Edoardo Orabona 4, 70125 Bari, Italy

- Developing of an atomistic model of Neutral Beam Injectors (NBI) for nuclear fusion technology using a native fortran code for the simulations of Solid-Gas interaction.
- Theoretical determination of Molybdenum-Caesium interaction using Density Functional Theory (DFT), Coupled-Cluster (CC) and Møller-Plesset Perturbation Theory (MP2).
- Modelling of metal oxides through Molecular Dynamics simulations for studying the Phase Transition behaviour at different temperatures and compositions.
- Molecular Dynamics simulations of Aquaporin for studying water Diffusion and its chemical interaction through the Transmembrane channels inside the proteins.

Sep. 2011 – Dec. 2011

Bachelor Internship

University of Bari,
Via Edoardo Orabona 4, 70125 Bari, Italy

- Development of environment-friendly functionalization of Multi-Walled Carbon Nanotubes using Dimethyl-Dioxirane as oxidising agent.
- Oxidised-Surface analysis of Multi-Walled Carbon Nanotubes using Raman, Infra-Red (IR) spectroscopy and Scanning Electron Microscope (SEM).

SKILLS

Mother tongue Italian

Other languages

	UNDERSTANDING		SPEAKING		WRITING
	Listening	Reading	Spoken interaction	Spoken production	
English	B2	B2	C1	C1	B2
Spanish	B1	A2	A2	B1	A2
German	A2	A2	A1	A1	A2
French	A1	A1	A1	A1	A1

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

Computer Skills

- Programming Languages : Fortran, C/C++, Python, Javascript, Linux Shell, DOS Shell, Java, OpenCL, Visual Basic, Processing.
- Software Knowledge : LAMMPS, Matlab, Gromacs, GAMESS-US, Chem-Office, LabView, SPHYSICS, Swift App-Developer, Adobe After Effect, Photoshop, LaTeX, Arduino, Neural Network (Machine Learning).
- Web : HTML5, PhP, p5.js.

Certificates

- Parallel Computing : 23rd Summer School on Parallel Computing. July 14th - 25th 2014, CINECA, Rome, Italy.
- Molecular Dynamics : Efficient use of Moleular Dynamics simulation application in a HPC environment. November 17th - 19th 2014, CINECA, Bologna, Italy.
- Programming Languages C++ : Introduction to Scientific and Technical Computing in C++. March 4th - 6th 2015, CINECA, Segrate-Milan, Italy.
- MPI and OpenMP : Introduction to Parallel Computing with MPI and OpenMP. December 9th - 11th 2015, CINECA, Bologna, Italy.
- LabVIEW Core 1 : Successfully attended the LabVIEW Core 1 Course. June 29th - July 1st 2015, University of Brescia, Italy.
- LabVIEW Core 2 : Successfully attended the LabVIEW Core 2 Course. July 2th-3st 2015, University of Brescia, Italy.
- LabVIEW Developer : Successfully Certified as Associate Developer. July 22th 2015, University of Brescia, Italy.

Extracurricular Activities

- Astronomical Observation Activities : Castellana Grotte, Italy. Radio-Astronomy, Computer simulations and study of the Chemical Composition of Exoplanets. Annual public dissemination “Presentation : Curiosity about Exoplanets". (2012 - 2015)
- High School Chemical Analysis : Bari, Italy. “Determination of the Structure by X-Ray diffraction and Nuclear Magnetic Resonance". “Analysis of water and study of Chemical Phenomena inherent to the underground world". (2007 - 2008)

Awards

- 4th Place, Regional Chemistry Olympic Games. Italy (2007)
- 4th Place, Regional Chemistry Olympic Games. Italy (2008)
- 2nd Place, *VI* Italian National Competition of Chemistry. Italy (2008)

Reviewer

- Nature Scientific Report

PUBLICATIONS

Google Scholar Updated List : [Link]

- **A. Damone**, *et al.* Theoretical determination of the microstructure of Cs covering of Mo in negative ion sources for nuclear fusion applications. *Journal of Plasma Physics and Controlled Fusion.* **57**, 3, (2015) [Link].
- P. Poesio, **A. Damone**, O. K. Matar. Slip at liquid-liquid interfaces. *Journal of Physical Review Fluids.* **2**, 4, (2017) [Link].
- P. Poesio, **A. Damone**, O. K. Matar. A multiscale approach to interpret and predict the apparent slip velocity at liquid-liquid interfaces. *Journal of Physics: Conference Series.* **923**, 012003, (2017) [Link].
- **A. Damone**, P. Poesio. Transport Properties of Water-Triethylamine Fluid Mixtures using Molecular Dynamics. *Journal of Chemical Engineering Data.* **64**, 9, 3731-3741 (2019) [Link].
- G. J. Wang, **A. Damone**, F. Benfenati, N. G. Hadjiconstantinou, P. Poesio, G. P. Beretta. Physics of nanoscale immiscible fluid displacement. *Journal of Physical Review Fluids.* **4**, 124203 (2019) [Link].
- T. Vo, B. Reeder, **A. Damone**, P. Newell. Simulation domain-size and boundary condition effect on mechanical response of amorphous silica: A reactive molecular dynamics study. *Nanomaterials. 10* (1), **54** (2020) [Link].
- A. M. Kulkarni, E. J. García, **A. Damone**, M. Schappals, S. Stephan, M. Kohns, H. Hasse. A Force-Field for Poly(Oxymethylene) Dimethyl Ethers (OMEs). *Journal of Chemical Theory and Computation. 16*, **4** (2020) [Link].
- P. Weingart, P. Hütchen, **A. Damone**, M. Kohns, H. Hasse, W. R. Thiel. Two simple and highly efficient variants of the Griffith-Ley oxidation of alcohols. *The European Society Journal of Catalysis - Chem. Cat. Chem.* (2020) [Link].
- T. Vo, B. He, M. Blum, **A. Damone**, P. Newell. Molecular scale insight of pore morphology relation with mechanical properties of amorphous silica using ReaxFF. *Computational Material science* **183**, 109881 (2020) [Link].

CONFERENCES

- ***Conference Collaborator***. Effect of Fluid on Crack Propagation in Amorphous Silica by Molecular Simulation. *American Geophysical Union, Fall Meeting 2019.* San Francisco, CA, U.S.A. (2019).
- ***Poster Presentation***. A transferable force field for Poly(oxymethylene) Dimethyl Ethers. *Thermodynamik Kolloquium Conference - DECHEMA.* Kassel, Germany (2018).
- ***Poster Presentation***. Hybrid-Atomistic Continuum Modelling of Liquid-Liquid Interfaces. *European Congress and Exhibition on Advanced Materials and Processes - EUROMAT.* Thessaloniki, Greece (2017).
- ***Conference Presenter***. Determining Transport Properties of Water-Triethylamine mixtures by Molecular Dynamics. *5th Micro and Nano Flows Conference.* Milan, Italy (2016).
- ***Conference Collaborator***. Predicting apparent slip at liquid-liquid interfaces without an interface slip condition. *68th Annual Meeting of the APS Division of fluid Dynamics.* Boston, MA, U.S.A. (2015).
- ***Conference Collaborator***. Ab-initio modelling of Cs-Mo interfaces in negative ion sources. *International Conference on Phenomena in Ionized Gases (ICPIG).* Iasi, Romania (2015).
- ***Conference Collaborator***. Molecular Dynamics of Plasma - Wall Materials for Fusion Technology. *International Conference on Phenomena in Ionized Gases (ICPIG).* Granada, Spain (2013).

Place and Date

Rueil-Malmaison 01/06/2020

Signature