Cristina Caruso

EDUCATION AND TRAINING

[11/2021 – Current] **Ph.D. Candidate in Materials Science and Technology (XXXVII Cycle)**

Politecnico di Torino

Investigation of complex dynamical systems using advanced computational approaches. Molecular modeling, molecular dynamics simulations and time-dependent descriptors are combined to study systems with non-trivial internal dynamics and emergent behaviors.

[05/2021 – 10/2021] **Pre-Ph.D. Fellow**

Politecnico di Torino

Development of automatic optimization tools for molecular models.

[10/2018 – 12/2020] **MSc Degree in Biomedical Engineering**

Politecnico di Torino

| **Final grade:** Cum Laude

Orientation: Bionanotechnologies

[09/2015 – 10/2018] **BSc Degree in Biomedical Engineering**

Politecnico di Torino

[2010 – 2015] **Diploma of Classical Maturity**

Liceo Classico IISS F. De Sanctis

WORK EXPERIENCE

[10/2023 – 03/2024] **Visiting Ph.D. Student**

Northwestern University, Department of Materials Science and Engineering

City: Evanston, IL 60208 | **Country:** United States

Study of ionic transport mechanisms through the crystalline domain of a ladder n-type polymer (poly-benzimidazobenzophenanthroline) for next-generation organic electrochemical transistors. DFT, molecular dynamics simulations and advanced molecular descriptors have been combined.

[03/2020 – 07/2020] **Master Thesis Student**

IDSIA, Department of Innovative Technologies

City: Lugano | **Country:** Switzerland

Thesis title: "Prediction of Drug-Target Unbinding Kinetics by Molecular Simulations".

Development of a novel computational approach enabling a reliable protein-ligand unbinding kinetics prediction. Enhanced sampling molecular dynamics simulations have been combined with dissociation pathways prediction algorithms.

LANGUAGE SKILLS

Mother tongue(s): Italian **Other language(s):** English (C1)

TECHNICAL SKILLS

Python programming

GROMACS

Experience with HPC environments

Basic knowledge of MATLAB/Simulink, C

Basic knowledge of COMSOL Multiphysics

CERTIFICATIONS AND COURSES

International Test of English Proficiency (iTEP), C1 (2023)

Mathematics for Machine Learning: Multivariate Calculus, Coursera, Imperial College London (2023)

Mathematics for Machine Learning: Linear Algebra, Coursera, Imperial College London (2022)

PUBLICATIONS

1. Classification and spatiotemporal correlation of dominant fluctuations in complex dynamical systems

C. Caruso, M. Crippa, A. Cardellini, M. Cioni, M. Perrone, M. Delle Piane and G. M. Pavan*, PNAS Nexus, pgaf038, (2025). DOI:10.1093/pnasnexus/pgaf038

2. TimeSOAP: tracking high-dimensional fluctuations in complex molecular systems via time-variations of SOAP spectra

C. Caruso, A. Cardellini, M. Crippa, D. Rapetti and G. M. Pavan*, J. Chem. Phys. 158, 214302 (2023). DOI:10.1063/5.0147025

3. Detecting dynamic domains and local fluctuations in complex molecular systems via timelapse neighbors shuffling

M. Crippa, A. Cardellini, **C. Caruso** and G. M. Pavan*, Proc. Natl. Acad. Sci. USA 2023, 120, e2300565120. DOI:10.1073/2300565120

4. Automatic optimization of lipid models in the Martini force field using SwarmCG

C. Empereur-mot*, K. B. Pedersen, R. Capelli, M. Crippa, **C. Caruso**, M. Perrone, P. C. T. Souza, S. J. Marrink and G. M. Pavan*, J. Chem. Inf. Model. 2023, 63, 12, 3827-3838. DOI: 10.1021/3c00530

5. Automatic multi-objective optimization of coarse-grained lipid force fields using SwarmCG

C. Empereur-mot*, R. Capelli, M. Perrone, **C. Caruso**, G. Doni and G. M. Pavan*, J. Chem. Phys. 156, 024801 (2022). DOI: 10.1063/5.0079044

CONTRIBUTION TO INTERNATIONAL CONFERENCES

1. Gordon Research Conference: Electronic Processes in Organic Materials, Lucca (Barga), July 7-12, 2024

Poster Presentation: *Toward fundamental ionic mechanisms underlying mixed ionic-electronic conductors for next-generation materials*, **C. Caruso**, F. Jimenez-Angeles, D. Meli, R. Wu, A. Cardellini, J. Rivnay, G. M. Pavan and M. Olvera de la Cruz

2. XLIX Congress of the Physical Chemistry Division of the Società Chimica Italiana, Torino (Italy), September 4-7, 2023

Oral contribution: *Tracking high-dimensional fluctuations in complex molecular systems via time-variations of local environments*, **C. Caruso**, A. Cardellini, M. Crippa, D. Rapetti and G. M. Pavan

3. CCP5 Summer School: Methods in Molecular Simulation, 28th Edition, Durham University, July 16-27, 2023

Poster presentation: *Tracking high-dimensional fluctuations in complex molecular systems via time-variations of local environments*, **C. Caruso**, A. Cardellini, M. Crippa, D. Rapetti and G. M. Pavan

4. Gordon Research Conference: Self-Assembly and Supramolecular Chemistry, Les Diablerets (Switzerland), May 14-19, 2023

Poster presentation: *Tracking high-dimensional fluctuations in complex molecular systems via time-variations of local environments*, **C. Caruso**, A. Cardellini, M. Crippa, D. Rapetti and G. M. Pavan

5. Gordon Research Seminar: Self-Assembly and Supramolecular Chemistry, Les Diablerets (Switzerland), May 13-14, 2023

Poster presentation: *Tracking high-dimensional fluctuations in complex molecular systems via time-variations of local environments,* **C. Caruso**, A. Cardellini, M. Crippa, D. Rapetti and G. M. Pavan

6. EuChemS 2022, Lisbon (Portugal), 28 August - 1 September, 2022

Poster presentation: *Towards the automatic design of density-responsive chemotactic nanoparticles,* **C. Caruso**, A. Cardellini, C. Empereur-mot, A. Tarzia, C. Lionello and G. M. Pavan

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Torino, 28/02/2025

Cristina Caruso