

Alan Ianeselli

computational scientist, biophysicist

Born in Bolzano (Italy) in 1992

Languages: italian (native), english (professional), german (C1)

E-mail: alan.ianeselli@gmail.com

Phone: +14752415061

Personal website: <https://alan.ianeselli.com/>



BIO

I am a Postdoctoral Associate at the University of Yale, New Haven (USA), in the Bioinformatics lab of Prof. Mark Gerstein.

I graduated (110 *cum laude*) in molecular biotechnology at the University of Trento (Italy, 2016), and received my PhD with *Summa Cum Laude* (very rare distinction in Germany, < 1%) in physics at the prestigious Ludwig-Maximilian University of Munich (Germany, 2022).

During my young career, I already received several awards, such as the PhD award in the Origin of Life field, the Young Researcher Award of the area north Italy + Austria, the Junior Research Award South Tyrol, two publication awards, one best talk award and an award for outstanding academic results.

I am author of 15 publications, many of which have been published in the highest rank journals such as Nature Chemistry, Nature Physics, Nature Review Physics, JACS.

I have a multidisciplinary research background, ranging from molecular dynamics, the physics of the origin of life, molecular biology, microscopy, chemometrics, machine learning and artificial intelligence. This has allowed me to tackle my scientific research from different perspectives and enrich it with heterogeneous methods.

My current research focuses on the following aspects:

-AI for structural biology and drug discovery: I apply machine learning techniques and develop advanced algorithms for the simulation of protein structures, integrating MD calculations with the most recent machine learning and AI tools (e.g. **AlphaFold 2**). In this way, I aim to enhance the exploration of biologically relevant structures and improve their drug targeting possibilities. I also develop methods for the analysis of protein conformations, such as approximated free energy reconstruction, clustering, and identification of conformational transitions.

-chemometrics: I develop scientific analysis algorithms for experimental chemical processes, integrating advanced mathematical and machine learning methods, in order to create complete analysis pipelines. I also embed them into softwares with a user-friendly graphical interface to be used by experimentalists for the analysis of chemical data in the most efficient way.

-data science for biology: I make use of the state-of-the-art computational technologies to analyze data of biological relevance. For example: analysis of microscopy images for FRET and co-localization, prediction of future outcomes from clinical data, modeling of DNA replication processes, dimensionality reduction of business data.

I am lecturer of the course of “Fundamentals of Programming in Python”, and teacher of the course “AI methods to manage and exploit business data”.

EDUCATION AND WORK EXPERIENCE

- 12.2023 – Ongoing **Postdoctoral Associate** (Yale University, New Haven, USA), Gerstein lab, Molecular Biophysics and Biochemistry [computational biophysics].
- 03.2022 – 12.2023 **Researcher** (Free University of Bozen-Bolzano, Italy, NOI Techpark) [computational sciences].
- 09.2017 – 04.2022 **PhD in Physics, Summa Cum Laude** (Ludwig-Maximilians-Universität München, Germany), lab of Prof. Dieter Braun, system's biophysics [physics of the origin of life]. Thesis: <https://doi.org/10.5282/edoc.29754>
- 01.2017 – 06.2017 **Research Fellow** (University of Trento, Italy), lab of Prof. Emiliano Biasini, molecular biophysics [molecular dynamics of the prion's folding intermediates].
- 09.2014 – 10.2016 **Master in Molecular Biotechnology, 110/110 e Lode** (University of Trento, Italy). Thesis with Prof. Pietro Faccioli, computational biophysics [molecular dynamics of the lysozyme protein].
- 08.2015 – 09.2015 **Research Fellow** (Laimburg Research Center, Bolzano, Italy), lab of Dr. Katrin Janik, functional genomics [DNA sequence analysis of eukaryotic pathogens of the apple plant].
- 09.2011 – 09.2014 **Bachelor in Molecular Biotechnology, 103/110** (University of Trento, Italy). Thesis with Prof. Yuri Bozzi, neurobiology [neurotrophic factors on the growth of neurons of autistic mice].

AWARDS

- 12.2023 **Junior Research Award Südtirol** by the Autonomous Provinz Bozen (Italien), 2nd prize 7500 €.
- 11.2022 **PhD Award** by the Excellence Cluster ORIGINS, (Deutsche Forschungsgemeinschaft DFG, Germany), prize 2000 €.
- 08.2022 **Young Researcher Award** by EUREGIO Tyrol (Austria) – South Tyrol (Italy) – Trentino (Italy), European Forum Alpbach (1st prize, 5000 €).
- 12.2019 **Publication Award** by CeNS (Center for NanoScience, LMU München). Best interdisciplinary publication.
- 07.2019 **Very important paper (VIP) award** by the journal Angewandte Chemie (5% of the best papers of the year).
- 09.2017 **PhD fellowship** awarded on a competitive basis by the graduate school of Quantitative Biosciences Munich (QBM).
- 08.2017 **Merit award** for outstanding academic results (prize 1200 €, awarded by the Province of Bolzano).
- 05.2017 **Merit award** for excellent academic results (prize 1300 €, awarded by the University of Trento).
- 08.2014 **Scholarship** for particular merits (summer internship at Laimburg Research Center, Italy, awarded by the Province of Bolzano).

PROGRAMMING LANGUAGES

- **Python:** advanced (8+ years of experience)
matplotlib, numpy, scipy, os, sys, libtiff, opencv, scikit-learn, tensorflow, ssh
- **LabVIEW:** advanced (5+ years of experience)
NI-DAQmx, IMAQdx, IMAQ, data analysis, property nodes, graphical interfaces

MD PROGRAMS

- Molecular visualization (VMD, Chimera)
- Molecular dynamics simulations (GROMACS, PLUMED)
- Computer clusters and remote connections (ssh)
- MD analysis scripts: change point analysis, clustering, path similarity, calculation of collective variables...

EXPERIMENTAL

- Microscope assembly: optics, electronics and hardware programming
- DNA replication (PCR, isothermal replication), poly-acrylamide and agarose gel electrophoresis
- Fluorescence microscopy imaging (SNARF-1, BCECF, Lysosensor, FRET)

MY SOFTWARES (short video tutorials at: <https://alan.ianeselli.com/software/>)

- **Chemometric analysis of wine chromatograms:** user-friendly graphical analysis software for the processing, alignment and quantification of multi-dimensional wine chromatograms, to strongly speed-up experimental analyses.
- **Image analysis (FRET):** interactive analysis of microscopy images for the calculation of DNA hybridization in bulk aqueous solutions.
- **RNA melting point calculator:** calculator of the melting temperature of complementary RNA duplexes, as a function of strand length, composition and water pH, temperature and salinity, based on experiments. Downloadable at the following link: <https://cloud.physik.lmu.de/index.php/s/CrGfsxqNZCDNRqr> (needs LabVIEW Runtime Engine 2014, which is free).
- **Simulator of DNA evolution:** Monte Carlo simulation of DNA replication under non-equilibrium forces, where DNA molecules replicate following a melting energy landscape.

TEACHING ACTIVITIES

- **Lecturer** for the course of “Fundamentals of Programming”, bachelor in Electronics and Cyber-Physical Systems Engineering, Free University of Bozen-Bolzano (March - June 2023).
- **Lecturer** for the course “Artificial Intelligence to manage and exploit business data”: training course funded by the European Social Fund 2022 (ESF30711) (3 sessions: September 2022; November 2022; February 2023)
- **Experimental physics training (“Praktikum”) for Master students (2 sessions, 3 students each).** 1 week of practical work experience for investigating the “non-equilibrium processes in the origin of life”, Ludwig Maximilians University München (2019 - 2021).
- **Supervision of (2) Bachelor students’ thesis project.** Ludwig-Maximilians-Universität München (2019, 2020). The students have been added in the authors list in my Nature Physics and Nature Chemistry paper.

OUTREACH

- **Presenter** at the “Open Day for Schools”, presentation of my research activities to highschool students. NOI Techpark, March 2nd, 2023; May 31st, 2022.
- **Presenter** during the lab visit of highschool student at NOI Techpark. Presentation of Smart Data Factory, February 9th 2023.
- **Presenter** at the event “Sfruttare il potenziale - Digital Technologies”, presentation of my advanced software for the graphical analysis of wine chromatograms, to private companies and freelancers. NOI Techpark, October 20th 2022.
- **Presenter** at the “Tag der Offenen Tür”, to present my work and the research projects of my lab to the public. Ludwig-Maximilians-Universität München, March 23rd, 2019.

GIVEN TALKS

- **SFSCON Free Software Conference 2023.** *Bolzano, NOI Techpark (Italy)*. Title: Machine learning-driven simulation of protein folding atomistic trajectories. November 10th 2023.
- **ORIGINS Excellence Cluster, Science Week 2022.** *Kloster-Seeon (Germany)*. Title: Hadean water-dew cycles drive the evolution of DNA and protocells. November 28th - December 1st 2022. **Best PhD Award**.
- **EUREGIO Young Researcher Award 2022.** *European Forum Alpbach (Tirol, Austria)*. Title: Water cycles drive DNA replication and evolution. August 19th - 21st, 2022. **Winner (1st prize)**
- **ORIGINS Excellence Cluster, Science Week 2019.** *Max Planck Institute for Extraterrestrial Physics, Garching (Germany)*. Title: Strand separation and replication of oligonucleotides in a primordial CO₂ atmosphere. December 4th, 2019.
- **CRC (Collaborative Research Center) Emergence of Life, Summer School 2019.** *Jugendherberg Regensburg (Germany)*. Title: DNA Denaturation Induced by Salt Fluctuations in a Microfluidic Water Cycle. June 6th, 2019.
- **QBM (Quantitative Biosciences Munich) Retreat 2019.** *Evangelische Akademie Tutzing (Germany)*. Title: DNA Denaturation Induced by Salt Fluctuations in a Microfluidic Water Cycle. June 12th – 14th, 2019. **Best talk award**

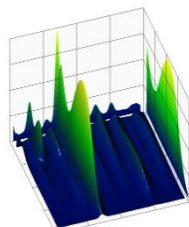
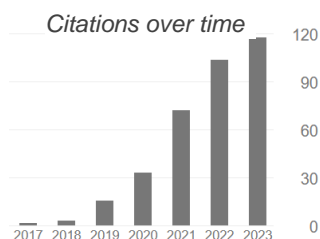
PUBLISHED PAPERS

As of December 2023:

Total citations = 351

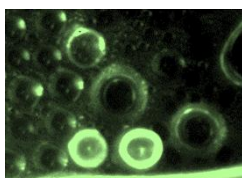
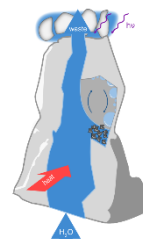
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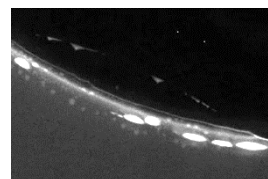
1. **laneselli, A.**; Longo, E.; Poggesi, S.; Montali, M.; Boselli, E. A complete analysis pipeline for the processing, alignment and quantification of HPLC-UV wine chromatograms. **2023**, accepted in *Chromatographia*. [impact factor 1.7]

2. **laneselli, A.**; Salditt, A.; Mast, C.; Ercolano, B.; Kufner, C.; Scheu, B.; Braun, D. Physical non-equilibria for prebiotic nucleic acid chemistry. *Nature Review Physics*, **2023**. <https://doi.org/10.1038/s42254-022-00550-3> [impact factor 36.2]



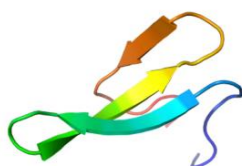
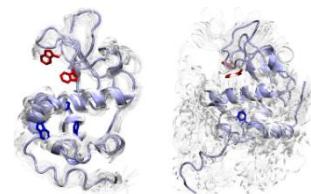
3. **laneselli, A.**; Atienza, M.; Kudella, P.; Mast, C.; Gerland, U.; Braun, D. Water cycles in a Hadean CO₂ atmosphere drive the evolution of long DNA. *Nature Physics*, **2022**. <https://doi.org/10.1038/s41567-022-01516-z> [impact factor 20.0]

4. **laneselli, A.**; Tetiker, D.; Stein, J.; Kühnlein, A.; Mast, C.; Braun, D.; Tang, D. T.-Y.; Non equilibrium conditions inside rock pores drive fission, maintenance and selection of coacervate protocells. *Nature Chemistry*, **2021**. <https://doi.org/10.1038/s41557-021-00830-y> [impact factor 24.4]



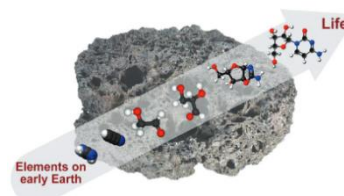
5. **laneselli, A.**; Mast, C.; Braun, D. Periodic melting of oligonucleotides by oscillating salt concentrations triggered by microscale water cycles inside heated rock pores. *Angewandte Chemie International Edition*, **2019**. *Very important paper*. <https://doi.org/10.1002/anie.201907909> [impact factor 15.3]

6. **laneselli, A.**; Orioli, S.; Spagnolli, G.; Faccioli, P.; Cupellini, L.; Jurinovich, S.; Mennucci, B. Atomic detail of protein folding revealed by an ab initio reappraisal of circular dichroism. *Journal of American Chemical Society*, **2018**. <https://doi.org/10.1021/jacs.7b12399> [impact factor 15.4]

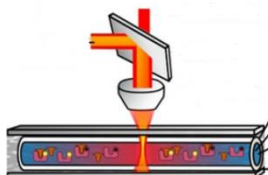
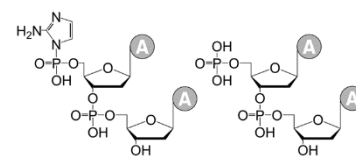


7. **laneselli, A.***; Orioli, S.*; Spagnolli, G.*; Faccioli, P. * = Equal contributions. All-atom calculation of protein free-energy profiles. *The Journal of Chemical Physics*, **2017**. <https://doi.org/10.1063/1.5006039> [impact factor 3.5]

8. Mast, C.; Langlais, J.; Wunnawa, S.; Serrao, A.; **laneselli, A.**; Matreux, T.; Weingart, M.; Dirscherl, C.; Salditt, A.; Braun, D. Emergence of life in the lab? *Bunsen Magazin*, **2022**. [10.26125/ac99-jt74](https://doi.org/10.26125/ac99-jt74)

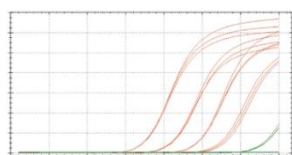
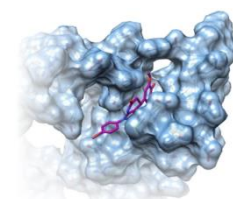


9. Dirscherl, C. F.; **laneselli, A.**; Tetiker, D.; Matreux, T.; Queener, R. M.; Mast, C.; Braun, D. A heated rock crack captures and polymerizes primordial DNA and RNA. *Physical Chemistry Chemical Physics*, 2022. <https://doi.org/10.1039/D2CP04538A> [impact factor 3.9]



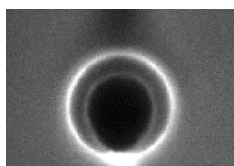
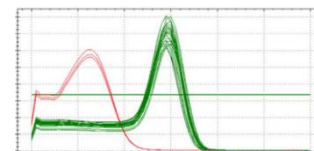
10. Stein, J. A. C.; **laneselli, A.**; Braun, D. Kinetic microscale thermophoresis for simultaneous measurement of binding affinity and kinetics. *Angewandte Chemie International Edition*, 2021. <https://doi.org/10.1002/anie.202101261> [impact factor 15.3]

11. Spagnoli, G.; Massignan, T.; Astolfi, A.; Biggi, S.; Rigoli, M.; Brunelli, P.; Libergoli, M.; **laneselli, A.**; Orioli, S.; Boldrini, A.; et al. Pharmacological inactivation of the prion protein by targeting a folding intermediate. *Communications Biology*, 2021. <https://doi.org/10.1038/s42003-020-01585-x> [impact factor 6.3]



12. Mittelberger, C.; Obkircher, L.; Oberkofler, V.; **laneselli, A.**; Kerschbamer, C.; Gallmetzer, A.; Reyes-Dominguez, Y.; Letschka, T.; Janik, K. Development of a universal endogenous qPCR control for eukaryotic DNA samples. *Plant Methods*, 2020. <https://doi.org/10.1186/s13007-020-00597-2> [impact factor 5.0]

13. Mittelberger, C.; Obkircher, L.; Oberkofler, V.; **laneselli, A.**; Kerschbamer, C.; Janik, K. Development of an endogenous universal internal control for qPCR applications and the importance of different evaluation criteria. *Phytopathogenic Mollicutes*, 2019. <http://dx.doi.org/10.5958/2249-4677.2019.00039.2> [impact factor 0.3]



14. Morasch, M.; Liu, J.; Dirscherl, C. F.; **laneselli, A.**; Kühnlein, A.; Le Vay, K.; Schwintek, P.; Islam, S.; Corpinot, M. K.; Scheu, B.; et al. Heated gas bubbles enrich, crystallize, dry, phosphorylate and encapsulate prebiotic molecules. *Nature Chemistry* 2019. <https://doi.org/10.1038/s41557-019-0299-5> [impact factor 24.4]

15. Wang, F.; Orioli, S.; **laneselli, A.**; Spagnoli, G.; a Beccara, S.; Gershenson, A.; Faccioli, P.; Wintrode, P. L. All-atom simulations reveal how single-point mutations promote serpin misfolding. *Biophysical Journal* 2018, 114 (9), 2083–2094. <https://doi.org/10.1016/J.BPJ.2018.03.027> [impact factor 4.0]

