ALLEGATO B

UNIVERSITÀ DEGLI STUDI DI MILANO
selezione pubblica per n.1 posto/i di Ricercatore a tempo determinato ai sensi dell'art.24, comma 3, lettera b) della Legge 240/2010 per il settore concorsuale 02/D1 - Fisica Applicata, Didattica e Storia della Fisica ,
settore scientifico-disciplinare FIS/07 - Fisica Applicata (a Beni Culturali, Ambientali, Biologia e Medicina)
presso il Dipartimento di Dipartimento di FISICA "ALDO PONTREMOLI" (avviso bando pubblicato sulla G.U. n. 53 del 05/07/2019) Codice concorso 4132

SANDRO BOTTARO
CURRICULUM VITAE

INFORMAZIONI PERSONALI (NON INSERIRE INDIRIZZO PRIVATO E TELEFONO FISSO O CELLULARE)

COGNOME	**BOTTARO**
NOME	**SANDRO**
DATA DI NASCITA	27/10/1983

INSERIRE IL PROPRIO CURRICULUM
(non eccedente le 30 pagine)

Data 27/06/2019 Luogo Milano

SANDRO BOTTARO

POSTDOCTORAL RESEARCH FELLOW

PERSONAL DETAILS

Born in Milan, Italy on October 27th, 1983

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ABOUT ME

I am a **theoretical physicist** working in the field of **computational biology**. I develop and apply computational methods with the aim of understanding the relationship between structure, dynamics, and function in biomolecules. I also develop methods to integrate computer simulations and experimental data to tackle problems for which experiment or computation alone do not provide an answer.

The final goal of my research is to provide powerful, robust, and **predictive computational tools** to advance our understanding of biological processes, to rationally design drugs and to gain mechanistic insights into disease-causing genetic mutations.

My expertise spans a variety of techniques, including molecular dynamics, Monte Carlo simulations, and enhanced sampling methods. My most recent interest is to employ machine learning approaches (e.g. unsupervised learning algorithms and **deep neural networks**) to tackle open challenges in computational modeling of biomolecules and materials.

POSTDOCTORAL EXPERIENCE

September 2018-present

Italian Institute of Technology, Genova, Italy and ETH Zurich, Switzerland

Department of Chemistry and Applied Biosciences

PI: Prof. Michele Parrinello

- Applications of deep neural networks and machine learning to atomistic simulations
- Computational Drug Discovery

2016-2018

University of Copenhagen, Copenhagen, Denmark

Structural Biology and NMR Laboratory

PI: Prof. Kresten Lindorff-Larsen

- Integrative structural biology
- Structural bioinformatics
- Analysis of RNA multiple sequence alignments

2012-2016

Scuola Internazionale Superiore di Studi Avanzati Trieste, Italy

Molecular and Statistical Biophysics group

- Free-energy calculations and enhanced sampling techniques
- Molecular Dynamics and Monte Carlo simulations

EDUCATION

PhD **Danish Technical University,** 2009-2012
Doctoral degree in computational Biophysics.

PhD **Cambridge University**, 2011
Visiting PhD student, Department of Chemistry.

MSc **Università degli Studi di Milano**, 2006-2009
MSc in theoretical Physics.
110/110 *Cum Laude*

BSc **Università degli Studi di Milano**, 2002-2006
BSc in Physics. *104/110*

PROGRAMMING

Python, C/C++, Bash, Latex

Python scientific libraries (NumPy, SciPy, Matplotlib, Jupyter, Sklearn, Keras, Tensorflow, Pandas)

User of high-performance cluster (HPC) facilities, graphical processing units (GPU), and related parallel software

SOFTWARE (as a developer)

- baRNAba - Python software package for analysis of RNA/DNA three-dimensional structures and simulations. https://github.com/srnas/barnaba
- Bayesian/MaxEnt refinement - Python library for integrative structural biology. https://github.com/KULL-Centre/BME
- HLDA - Python routine to perform linear discriminant analysis. https://github.com/sbottaro/HLDA
- PLUMED - plugin for free-energy calculations. https://www.plumed.org/
- PHAISTOS - Monte Carlo protein simulation framework. http://www.phaistos.org

INTERNATIONAL COLLABORATIONS

- **Douglas H. Turner.** *University of Rochester, New York (USA)*
- **Hashim Al-Hashimi.** *Duke University, North Carolina (USA)*
- **Thomas Cheatam.** *University of Utah, Utah (USA)*
- **Jiri Sponer**. *University of Prague, Czech Republic*
- **Pavel Banáš**. *Olomouc University, Czech Republic*

HABILITATION

Abilitazione Scientifica Nazionale from 10/04/2018; Settore concorsuale 02/D1 (Fisica applicata, didattica e storia della Fisica), SSD FIS/07

MENTORING EXPERIENCE

PhD students:

- Xiaohui Wang. *ETH Lugano* (2018-2019)
- Tone Bengtsen and Mustapha Carab. *Copenhagen University* (2016-2018).
- Giovanni Pinamonti. *SISSA* (2013-2015).
- Andrea Perez Villa. *SISSA* (2013-2014).
- Francesco di Palma. *SISSA* (2012-2013).

Master's students:

Marco Jacopo Ferrarotti. *International Master Course in Physics of Complex Systems, SISSA*. (2012)

TEACHING EXPERIENCE

2011: Teaching assistant, course in Tissue Biomechanics, Danish Technical University, Denmark.

2013-2015: Teaching assistant, Summer School on Atomistic Simulation Techniques for Material Science, Nanotechnology and Biophysics. SISSA, Trieste, Italy

2016: Lecturer at Master in High Performance Computing at ICTP/SISSA, Trieste, Italy.

REVIEWING ACTIVITY

Peer reviewer for the following journals:

- Journal of the American Chemical Society; PLoS Computational Biology; Genes; Bioinformatics; Living Journal of Computational Molecular Science; Frontiers in Molecular Biosciences; Journal of Computer Aided Molecular Design; BMC Bioinformatics; Biochemistry

Publons ID: publons.com/a/1290569/

INTERNATIONAL TALKS (selected list)

June 2018. TSRC Workshop on Protein Dynamics. *École de Physique des Houches, France.*

July 2017. RNA Dynamics Workshop. *Telluride Science Research Center. Telluride, Colorado, USA*.

March 2017. Towards a Quantitative Understanding of Life Machinery. *International Center for Theoretical Physics, Trieste, Italy.*

Feb 2017. Physics of Protein Folding and Aggregation. *Bressanone, Italy.*

PUBLICATION LIST

STATISTICS

Documents:	24 (28)	h-index:	14 (17)
Citations:	470 (658)	Total impact factor:	225 (na)

Source: SCOPUS (Google Scholar)

FIRST AUTHOR PAPERS

1. **Molecular Dynamics Simulations, Exact NOE Measurements, and Machine Learning Reveal a Low-populated State of the UUCG RNA Tetraloop**
   Bottaro S, Nichols P, Vögeli B, Parrinello M, Lindorff-Larsen K. *(Submitted manuscript)*
2. **Biophysical Experiments and Biomolecular Simulations: a Perfect Match?**
   Bottaro S, Lindorff-Larsen K.
   Science (2018)
3. **Barnaba: Software for Analysis of Nucleic Acids Structures and Trajectories**
   Bottaro S, Pinamonti G, Reisser S, Boomsma W, Lindorff-Larsen K, and Bussi G.
   RNA (2018)
4. **Integrating Molecular Simulation and Experimental Data: a Bayesian/MaxEnt (BME) reweighting approach**
   Bottaro S, Bengtsen T and Lindorff-Larsen K.
   Methods in Molecular Biology (2018)
5. **Conformational ensembles of RNA oligonucleotides from integrating NMR and molecular simulations**
   Bottaro S, Bussi G, Kennedy SD, Turner DH, Lindorff-Larsen K.
   Science Advances (2018)
6. **Mapping the Universe of RNA Tetraloop Folds**
   Bottaro S, Lindorff-Larsen K
   Biophysical Journal (2017)
7. **Free energy landscape of GAGA and UUCG RNA tetraloops**
   Bottaro S, Banáš P, Sponer J, and Bussi G.
   Journal of Physical Chemistry Letters (2016)
8. **RNA Folding Pathways in Stop Motion**
   Bottaro S, Gil-Ley A, and Bussi G.
   Nucleic Acids Research (2016)
9. **Towards RNA 3D Structure Prediction**
   Bottaro S, Di Palma F, and Bussi G.
   RNA and Disease (2015)
10. **The Role of Nucleobase Interactions in RNA Structure and Dynamics**
    Bottaro S, Di Palma F, and Giovanni Bussi.
    Nucleic Acids Research (2014)
11. **Variational Optimization of an All-Atom Implicit Force Field To Match Explicit Solvent Simulation Data**
    Bottaro S, Lindorff-Larsen K, and Best RB.
    Journal of Chemical Theory and Computation (2013)
12. **Subtle Monte Carlo Updates in Dense Molecular Systems**
    Bottaro S, Boomsma W, Enoe J. K, Andreetta C, Hamelryck T, and Ferkinghoff-Borg J.
    Journal of Chemical Theory and Computation (2012)

PUBLICATION LIST

CO-AUTHORED PAPERS

13. **The PLUMED consortium: A community effort to promote openness, transparency and reproducibility in molecular simulations**
    The PLUMED consortium
    (Submitted Manuscript)

14. **Fitting corrections to an RNA force field using experimental data**
    Cesari A, Bottaro S, Lindorff-Larsen K, Banáš P, Sponer J, Bussi G.
    Journal of Chemical Theory and Computation (2019)

15. **Effects and limitations of a nucleobase-driven backmapping procedure for nucleic acids using steered molecular dynamics**
    Poblete S, Bottaro S, and Bussi G.
    Biochemical and Biophysical Research Communications (2017)

16. **RNA Structural Dynamics as Captured by Molecular Simulations: A Comprehensive Overview**
    Sponer J, Bussi G, Miroslav K; Banáš P, Bottaro S, Cunha R, Gil-Ley A, Pinamonti G, Poblete S, Jurecka P, Walter N, Otyepka M.
    Chemical Reviews (2017)

17. **A nucleobase-centered Coarse-Grained Representation for Structure Prediction of RNA Motifs**
    Poblete S, Bottaro S, Bussi G.
    Nucleic Acids Research (2017)

18. **Computer Folding of RNA Tetraloops: Identification of Key Force Field Deficiencies**
    Kührová P, Best RB, Bottaro S, Bussi G, Sponer J, Otyepka M, and Banáš P.
    Journal of Chemical Theory and Computation (2016)

19. **Empirical corrections to the Amber RNA force field with Target Metadynamics**
    Gil-Ley A, Bottaro S, and Bussi G.
    Journal of Chemical Theory and Computation (2016)

20. **Elastic Network Models for RNA: A Comparative Assessment with Molecular Dynamics and SHAPE Experiments**
    Pinamonti G, Bottaro S, Micheletti C, Bussi G.
    Nucleic Acids Research (2015)

21. **Kissing Loop Interaction in Adenine Riboswitch: Insights from Umbrella Sampling Simulations**
    Di Palma F, Bottaro S, and Bussi G.
    BMC Bioinformatics (2015)

22. **Accurate Multiple Time Step in Biased Molecular Simulations**
    Ferrarotti J, Bottaro S, Perez-Villa A, Bussi G.
    Journal of Chemical Theory and Computation (2015)

23. **Formulation of Probabilistic Models of Protein Structure in Atomic Detail Using the Reference Ratio Method**
    Valentin J, Andreetta C, Boomsma W, Bottaro S, Ferkinghoff-Borg J, Frellsen J, Mardia KV, Pengfei T, Hamelryck T.
    Proteins (2014)

24. **PHAISTOS: A Markov Chain Monte Carlo Protein Simulation Framework**
    Boomsma W, Frellsen J, Harder T, Bottaro S, Enoe J. K, Pengfei T, Stovgaard K, Andreetta C, Borg M, Ferkinghoff-Borg J, Hamelryck T.
    Journal of Computational Chemistry (2013)

PUBLICATION LIST

25. An Efficient Null Model for Conformational Fluctuations in Proteins
    Harder T, Borg M, Bottaro S, Boomsma W, Olsson S, Ferkinghoff-Borg J, Hamelryck T.
    Structure (2012)

26. Generative Probabilistic Models Extend the Scope of Inferential Structure Determination
    Olsson S, Boomsma W, Frellsen J, Bottaro S, Harder T, Ferkinghoff-Borg J, Hamelryck T.
    Journal of Magnetic Resonance (2011)

27. Potentials of Mean Force for Protein Structure Prediction Vindicated, Formalized and Generalized
    Hamelryck T, Borg M, Paluszewski M, Paulsen J, Frellsen J, Andreetta C, Boomsma W, Bottaro S, and Ferkinghoff-Borg J.
    PLOS ONE (2010)

28. Accuracy of the Pseudopotential Approximation in ab initio Theoretical Spectroscopies
    Luppi E, Weissker H, Bottaro S, Sottile F, Veniard V, Reining L, and Onida G.
    Physical Review B (2008)