Curriculum Vitae of Giovanni Bussi

extended version

(updated October 28, 2025)

Personal informations

Name	Giovanni Bussi
Address	Scuola Internazionale Superiore di Studi Avanzati (SISSA) via Bonomea 265, 34136 Trieste, Italy
Telephone	+39 040 3787 407
Email	bussi@sissa.it giovanni.bussi@gmail.com
Web	http://people.sissa.it/~bussi http://bussilab.org

Education

- March 2005:
  Ph. D. in Physics, Università di Modena e Reggio Emilia, Italy.
  Thesis: *Excited states in low-dimensional systems.*
  Supervisors: Prof. Elisa Molinari and Dr. Alice Ruini.

- October 2001:
  Degree in Physics, Università di Modena e Reggio Emilia, Italy.
  Thesis: *Proprietà ottiche di polimeri coniugati*
  (Optical properties of conjugated polymers).
  Supervisors: Prof. Elisa Molinari and Dr. Alice Ruini.
  Mark: 110/110 *cum laude*.

Bibliographic metrics

- ISI Web of Science http://www.webofscience.com/wos/author/record/A-1776-2009
  - More than 100 records, collecting more than 24000 citations. H-factor: 43.
  - Five renowned papers ($\geq$500 citations).
  - Eight famous papers (250–499 citations).
  - Nine very well-known papers (100–249 citations).
- Google Scholar profile: http://scholar.google.it/citations?user=8qk_P2YAAAAJ

Professional experience

- Since February 2020:
  Full professor at SISSA, Trieste, Italy.
- March 2014 – January 2020:
  Associate Professor (tenured) at SISSA, Trieste, Italy.
- April 2011 – March 2014:
  Assistant professor (*Ricercatore a tempo determinato*) at SISSA, Trieste, Italy.
- September 2009 – April 2011:
  Research position at SISSA, Trieste, Italy.
- July 2008 – August 2009:
  Research position at the Università di Modena e Reggio Emilia, Italy.
- February 2005 – July 2008:
  Post-Doctoral position at the ETH Zürich in Computational Science, c/o the research group of Prof. Michele Parrinello, Lugano, Switzerland.
- November 2004 – December 2004:
  INFM Research Fellowship, *Electronic properties of nanotubes and other nanostructures*, Università di Modena e Reggio Emilia, Italy.
- January 2002 – December 2004:
  Ph. D. Fellowship, Università di Modena e Reggio Emilia, Italy.
- November 2001 – January 2002:
  INFM Research Fellowship, *Interazioni molecole organiche - superfici (Organic molecules - surface interactions)*, Università di Modena e Reggio Emilia, Italy.

Funding

- PRIN (2022) - *Hunting metal ions within cryo-EM derived RNA structures* ≈ 190k EUR, 97k EUR for SISSA unit.
- ERC Starting Grant (2012) - *Small RNAs in silico* ≈ 1300k EUR.
- MIUR FIRB (2011) *RNA modeling: folding, unfolding and switching,* ≈ 500k EUR.
- Young SISSA researcher grant (2011) *Pushing on PLUMED* ≈ 10k EUR.
- Thomas Young Center Junior Research Fellowship (2008), ≈ 1k GBP.
- Several grants for supercomputing access at CINECA within the ISCRA initiative.

Honors and awards

- MIUR Habilitation as Full Professor (2019) – 02/B2 (Fisica teorica della materia).
- MIUR Habilitation as Full Professor (2017) – 03/A2 (Modelli e metodologie per le scienze chimiche) and 02/D1 (Fisica applicata, didattica e storia della fisica).
- MIUR Habilitation as Full Professor (2014) – 02/B2 (Fisica teorica della materia).

- MIUR Habilitation as Associate Professor (2013) – 02/B2 (Fisica teorica della materia).
- Premio Città Impresa (2013).
- Premio Città Impresa (2012).

Institutional responsibilities

- 2023, Member of the EuroHPC regular access panel for Biochemistry, Bioinformatics and Life Sciences.
- 2020–2022, Member of the PRACE Access Committee.
- 2019–2022, Member of the scientific panel of the HPC-Europa3 funding scheme.
- 2016–2021 Coordinator of the PhD program in *Physics and Chemistry of Biological Systems*, SISSA, Trieste (Italy).

Research interests

I took my PhD at the Università di Modena and Reggio Emilia (Italy), under the supervision of Prof. Elisa Molinari. My research activity has been focused on the calculation of electronic and optical properties of low-dimensional systems, developing and applying methods taken from the solid state physics to study systems such as polymer crystals and carbon nanotubes. After the PhD, I moved to the ETH Zürich and I joined the group of Prof. Michele Parrinello. There, I worked on the development of methods for the simulation of rare events and on their applications to biological problems. In particular, I contributed several crucial improvements to a technique developed in the last decade in the Parrinello's group (metadynamics), an algorithm aimed at accelerating rare events in molecular dynamics simulations. Furthermore, I worked on the development of sampling algorithms for molecular dynamics, including a thermostating protocol that is currently my most cited work. When I started an independent activity my research interests gradually shifted towards development and application of computational techniques to RNA molecules. These activities have received national (FIRB) and international (ERC) fundings. My group is currently working on the *in silico* characterization of riboswitches and RNA/protein interactions and on the prediction of RNA structures. To this aim we develop new techniques, which are then published as open software. The group currently includes five PhD students and two post-docs. We develop and apply methods based on molecular dynamics, enhanced sampling techniques, coarse-grain models, structural bioinformatics, and analysis of experimental data to study RNA, the most intriguing actor of molecular biology.

Peer review

Reviewer for several high impact journals, including: Nature journals, Journal of the Americal Chemical Society, Nucleic Acids Research, Procs. Natl. Acad. Sci. U.S.A., Physical Review Letters, Journal of Physical Chemistry Letters, Journal of Chemical Theory and Computation, Journal of Physical Chemistry, Biochemistry, RNA Journal, Biophysical Journal, PLOS, Journal of Chemical Physics, Physical Review. Reviewer for several funding agencies, including ERC, FWF, NSF, EuroHPC, PRACE, and ISCRA.

Mentoring

- Giuseppe Sacco, PhD student, SISSA (since 2023), with Prof. Guido Sanguinetti (SISSA).
- Salvatore Di Marco, PhD student, SISSA (since 2023), with Dr. Alessandra Magistrato (CNR).
- Olivier Languin-Cattoën, post doc, SISSA (since 2023).
- Tomàs F.D. Silva, post doc, SISSA (since 2023).
- Elisa Posani, PhD student, SISSA (since 2022), with Dr. Alessandra Magistrato (CNR).
- Ivan Gilardoni, PhD student, SISSA (since 2022).
- Vittorio Del Tatto, undergraduate student, University of Trento (2021).
- Valerio Piomponi, PhD student, SISSA (2020–2023).
- Thorben Fröhlking, PhD student, SISSA (2019-2022).
- Mattia Bernetti, post doc, SISSA (2018–2021).
- Nicola Calonaci, PhD student, SISSA (2017–2020).
- Francesca Cuturello, PhD student, SISSA (2016–2019).
- Sabine Reißer, post doc, SISSA (2015–2018).
- Vojtech Mlýnský, post doc, SISSA (2015–2017).
- Simon Poblete, post doc, SISSA (2014–2018).
- Andrea Cesari, undergraduate student, Master in Physics of Complex Systems then PhD student, SISSA (2014–2018).
- Richard André Cunha, postgraduate student then PhD student, SISSA (2013–2017).
- Alejandro Gil-Ley, PhD student, SISSA (2013–2016).
- Giovanni Pinamonti, PhD student, SISSA (2013–2016).
- Marco Jacopo Ferrarotti, undergraduate student, Master in Physics of Complex Systems (2013).
- Pasquale Pisani, visiting PhD student, IIT, with Dr. Giovanni Bottegoni and Prof. Andrea Cavalli (2013–2014).
- Sandro Bottaro, post doc, SISSA (2012–2016).
- Maria Darvas, post doc, SISSA (2012–2015).
- Andrea Pérez Villa, PhD student, SISSA (2012–2015).
- Francesco di Palma, PhD student, SISSA (2011–2014).
- Francesco Colizzi, post doc, SISSA (2010–2013).

- Olaniyi Kamil Yusuff, PhD student, STEP program, ICTP, with Dr. Simone Raugei (2010–2011).
- Trang Do Nhu, PhD student, SISSA, with Prof. Paolo Carloni (2010–2012).

Teaching and dissemination

- January 2024:
  Lecturer for the course *RNA structure*, Ph.D. in Functional and Structural Genomics, SISSA, Trieste, Italy.
- October 2023–March 2024:
  Lecturer for the course *Theoretical foundations of molecular dynamics*, Ph.D. in Physics and Chemistry of Biological Systems, SISSA, Trieste, Italy.
- January 2023:
  Lecturer for the course *RNA structure*, Ph.D. in Functional and Structural Genomics, SISSA, Trieste, Italy.
- October 2022–March 2023:
  Lecturer for the course *Theoretical foundations of molecular dynamics*, Ph.D. in Physics and Chemistry of Biological Systems, SISSA, Trieste, Italy.
- January 2022:
  Lecturer for the course *RNA structure*, Ph.D. in Functional and Structural Genomics, SISSA, Trieste, Italy.
- October 2021–February 2022:
  Lecturer for the course *Theoretical foundations of molecular dynamics*, Ph.D. in Physics and Chemistry of Biological Systems, SISSA, Trieste, Italy.
- December 2020:
  Lecturer for the course *RNA structure*, Ph.D. in Functional and Structural Genomics, SISSA, Trieste, Italy.
- October 2020–February 2021:
  Lecturer for the course *Theoretical foundations of molecular dynamics*, Ph.D. in Physics and Chemistry of Biological Systems, SISSA, Trieste, Italy.
- December 2019:
  Lecturer for the course *RNA structure*, Ph.D. in Functional and Structural Genomics, SISSA, Trieste, Italy.
- October 2019–February 2020:
  Lecturer for the course *Theoretical foundations of molecular dynamics*, Ph.D. in Physics and Chemistry of Biological Systems, SISSA, Trieste, Italy.
- December 2018:
  Lecturer for the course *RNA structure*, Ph.D. in Functional and Structural Genomics, SISSA, Trieste, Italy.
- October 2018–February 2019:
  Lecturer for the course *Theoretical foundations of molecular dynamics*, Ph.D. in Physics and Chemistry of Biological Systems, SISSA, Trieste, Italy.
- November 2017–February 2018:
  Lecturer for the course *Theoretical foundations of molecular dynamics*, Ph.D. in Physics and Chemistry of Biological Systems, SISSA, Trieste, Italy.

- November 2017:
  Lecturer for the course *RNA structure*, Ph.D. in Functional and Structural Genomics, SISSA, Trieste, Italy.
- May 2017:
  Organizer and tutor for the "PLUMED Meeting 2017" SISSA, Trieste, Italy.
- November 2016–February 2017:
  Lecturer for the course *Theoretical foundations of molecular dynamics*, Ph.D. in Physics and Chemistry of Biological Systems, SISSA, Trieste, Italy.
- November 2016:
  Lecturer for the course *RNA structure*, Ph.D. in Functional and Structural Genomics, SISSA, Trieste, Italy.
- July 2016:
  Tutor and lecturer in *Molecular dynamics* for the CECAM "Summer school on atomistic simulation techniques," Trieste, Italy.
- November 2015–February 2016:
  Lecturer for the course *Theoretical foundations of molecular dynamics*, Ph.D. in Physics and Chemistry of Biological Systems, SISSA, Trieste, Italy.
- July 2015:
  Organizer, tutor and lecturer in *Molecular dynamics* for the CECAM "Summer school on atomistic simulation techniques for material science, nanotechnology and biophysics," Trieste, Italy.
- November 2014–February 2015:
  Lecturer for the course *Theoretical foundations of molecular dynamics*, Ph.D. in Physics and Chemistry of Biological Systems, SISSA, Trieste, Italy.
- July 2014:
  Organizer, tutor and lecturer in *Molecular dynamics* for the CECAM "Summer school on atomistic simulation techniques for material science, nanotechnology and biophysics," Trieste, Italy.
- May 2014:
  Organizer and tutor for the CECAM tutorial "Enhancing molecular simulations with PLUMED," Belfast, UK.
- November 2013–February 2014:
  Lecturer for the course *Theoretical foundations of molecular dynamics*, Ph.D. in Physics and Chemistry of Biological Systems, SISSA, Trieste, Italy.
- July 2013:
  Organizer, tutor and lecturer in *Molecular dynamics* for the CECAM "Summer school on atomistic simulation techniques for material science, nanotechnology and biophysics," Trieste, Italy.
- November 2012–February 2013:
  Lecturer for the course *Simulation of Biomolecules*, Ph.D. in Physics and Chemistry of Biological Systems, SISSA, Trieste, Italy.

- September 2012:
  Tutor and lecturer in *Molecular dynamics* and *Enhanced sampling methods* for the PASI school "Molecular-based Multiscale Modeling and Simulation," Montevideo, Uruguay.

- July 2012:
  Tutor and lecturer in *Molecular dynamics* for the CECAM "Summer school on atomistic simulation techniques for material science, nanotechnology and biophysics," Trieste, Italy.

- November 2011–February 2012:
  Lecturer for the course *Simulation of Biomolecules*, Ph.D. in Physics and Chemistry of Biological Systems, SISSA, Trieste, Italy.

- September 2011:
  Tutor and lecturer in *Metadynamics* and *Thermostats* for the "São Paulo Advanced school on Computational Materials Science for energy and environmental applications," São Paulo, Brazil.

- July 2011:
  Tutor and lecturer in *Molecular dynamics* for the CECAM "Summer school on atomistic simulation techniques for material science, nanotechnology and biophysics," Trieste, Italy.

- February 2011:
  Tutor in *Molecular dynamics: ensembles and thermostats* for the CECAM tutorial "2nd CP2K Tutorial: Enabling the Power of Imagination in MD Simulations," Zurich, Switzerland.

- January–March 2011:
  Lecturer for the course *Simulation of Biomolecules*, Ph.D. in Physics and Chemistry of Biological Systems, SISSA, Trieste, Italy.

- September 2010:
  Organizer and tutor for the CECAM tutorial "Free-energy calculations with PLUMED," Lausanne, Switzerland.

- July 2010:
  Tutor in *Molecular dynamics* for the CECAM "Summer school on atomistic simulation techniques for material science, nanotechnology and biophysics," Trieste, Italy.

- February 2010:
  Lecturer in *Theory and practice of density functional theory* for the school organized within the First International Workshop on Computational Biophysics (IWCBP-1), Ho Chi Minh City, Vietnam.

- January–March 2010:
  Lecturer for the course *Simulation of Biomolecules*, Ph.D. in Physics and Chemistry of Biological Systems, SISSA, Trieste, Italy.

- September 2008:
  Lecturer for part of the course *Simulation Methods: Molecular Dynamics*, Graduate School in Nano and Physical Sciences, Modena, Italy.

- February 2008:
  Lecturer for part of the course *Computational Structural Biology*, Corso di Perfezionamento, Scuola Normale Superiore, Pisa, Italy.

- November 2007:
  Lecturer for the ICTP-NMC School on Computational Condensed Matter Physics, Abuja, Nigeria.

- March 2007:
  Lecturer for part of the course *Computational Structural Biology*, Corso di Perfezionamento, Scuola Normale Superiore, Pisa, Italy.

- February–April 2004:
  Lecturer, Dipartimento di Fisica, Università di Modena e Reggio Emilia, Italy
  Esercitazioni per Elementi di Fisica dello Stato Solido
  (Exercises on Elements of Solid State Physics).

- June 2003:
  Lecturer in *Bethe-Salpeter equation* for the EXC!TiNG Summer School "DFT beyond the ground state", Riksgränsen, Sweden.

- December 2003:
  In charge of guided tour for the *Linus Pauling and the Twentieth Century* exhibit, hosted by INFM-S3, Modena, Italy.

- February–April 2003:
  Lecturer, Dipartimento di Fisica, Università di Modena e Reggio Emilia, Italy,
  Esercitazioni per Elementi di Fisica dello Stato Solido
  (Exercises on Elements of Solid State Physics).

Publications on Journals

Corresponding author is marked (*)

1. T. F.D. Silva*, **G. Bussi**
   Characterizing RNA oligomers using Stochastic Titration Constant-pH Metadynamics simulations
   Preprint: arXiv:2410.16064

2. S. Di Marco, J. Aupič*, **G. Bussi***, A. Magistrato*
   All-atom simulations elucidate the molecular mechanism underlying RNA-membrane interactions
   Submitted (2024)
   Preprint: bioRxiv doi:10.1101/2024.11.01.618995

3. E. Posani, P. Janos, D. Haack, N. Toor, M. Bonomi, A. Magistrato*, **G. Bussi***
   Ensemble Refinement of mismodeled cryo-EM RNA Structures Using All-Atom Simulations
   Submitted (2024)
   Preprint: bioRxiv doi:10.1101/2024.07.24.604258

4. R. Amaro, et al
   The need to implement FAIR principles in biomolecular simulations
   Submitted (2024)
   Preprint: arXiv:2407.16584

5. **G. Bussi***, M. Bonomi*, P. Gkeka*, M. Sattler*, et al
   RNA dynamics from experimental and computational approaches
   Structure 32, 1281 (2024)
   Preprint: arXiv:2404.02789

6. V. Piomponi*, M. Krepl, J. Šponer, and **G. Bussi***
   Molecular Simulations to Investigate the Impact of N6-Methylation in RNA Recognition: Improving Accuracy and Precision of Binding Free Energy Prediction
   J. Phys. Chem. B 128, 8896 (2024)
   Preprint: arXiv:2404.14821

7. B. C. Thiel, **G. Bussi**, S. Poblete*, I. L. Hofacker*
   Sampling globally and locally correct RNA 3D structures using ERNWIN, SPQR and experimental SAXS data
   Nucleic Acids Res. 52, e73 (2024)
   Preprint: bioRxiv doi:10.1101/2022.07.02.498583

8. V. V. Mykuliak*,R. Rahikainen, N. J. Ball, **G. Bussi**, B. T. Goult, V. P.Hytönen*
   Molecular dynamics simulations reveal how vinculin refolds partially unfolded talin rod helices to stabilize them against mechanical force
   PLoS Comput. Biol. 20, e1012341 (2024)

9. P. Pokorna, M. Mlýnský, **G. Bussi**, J. Šponer, and P. Stadlbauer*
   Molecular dynamics simulations reveal the parallel stranded d(GGGA)3GGG DNA quadruplex folds via multiple paths from a coil-like ensemble
   Int. J. Biol. Macromol. 261, 129712 (2024)
   Preprint: bioRxiv doi:10.1101/2023.09.09.556957

10. I. Gilardoni, T. Fröhlking, and **G. Bussi***
Boosting Ensemble Refinement with Transferable Force-Field Corrections: Synergistic Optimization for Molecular Simulations J. Phys. Chem. Lett. 15, 1204 (2024)
Preprint: arXiv:2311.13532

11. N. Calonaci, M. Bernetti, A. Jones, M. Sattler, **G. Bussi***
Molecular dynamics simulations with grand-canonical reweighting suggest cooperativity effects in RNA structure probing experiments
J. Chem. Theory Comput. 12, 3672 (2023)
Preprint: arXiv:2209.12640

12. T. Fröhlking, M. Bernetti, and **G. Bussi***
Simultaneous refinement of molecular dynamics ensembles and forward models using experimental data
J. Chem. Phys. 158, 214120 (2023)
Preprint: arXiv:2303.09372

13. Z. Zhang, J. Šponer, **G. Bussi**, V. Mlýnský, P. Šulc, C. R. Simmons, N. Stephanopoulos, and M. Krepl
Atomistic Picture of Opening–Closing Dynamics of DNA Holliday Junction Obtained by Molecular Simulations
J. Chem. Inf. Model. 26, 2794 (2023)

14. W.-T. Hsu, V. Piomponi, P. T. Merz, **G. Bussi**, and M. R. Shirts*
Adding alchemical variables to metadynamics to enhance sampling in free energy calculations
J. Chem. Theory Comput. 19, 1805 (2023)
Preprint: arXiv:2206.01329

15. M. Bernetti and **G. Bussi***
Integrating experimental data with molecular simulations to investigate RNA structural dynamics
Curr. Open. Struct. Biol. 78, 102503 (2023)
Preprint: arXiv:2207.08622

16. Biomotors, Viral Assembly, And RNA Nanobiotechnology: Current Achievements And Future Directions
L. Rolband, D. Beasock, Y. Wang, Y.-G. Shu, J. D. Dinman, T. Schlick, Y. Zhou, J. S. Kieft, S.-J. Chen, **G. Bussi**, A. Oukhaled, X. Gao, P. Šulc, D. Binzel, A. S. Bhullar, C. Liang, P. Guo*, K. A. Afonin*
Comput. Struct. Biotechnol. J. 20, 6120 (2022)

17. A. Dutta*, K. Tapio, A. Suma, A. Mostafa, Y. Kanehira, V. Carnevale, **G. Bussi**, and I. Bald*
Molecular states and spin crossover of hemin studied by DNA origami enabled single-molecule surface-enhanced Raman scattering
Nanoscale 14, 16467 (2022)

18. I. L. Grothaus, **G. Bussi**, and L. Colombi Ciacchi*
Exploration, Representation, and Rationalization of the Conformational Phase Space of N-Glycans
J. Chem. Inf. Model. 62, 4992 (2022)
Preprint: bioRxiv doi:10.1101/2022.06.17.496605

19. V. Piomponi, T. Fröhlking, M. Bernetti, and **G. Bussi***
Molecular Simulations Matching Denaturation Experiments for $N^6$6-Methyladenosine
ACS Cent. Sci. 8, 1218 (2022)
Preprint: arXiv:2203.14886

20. T. Fröhlking, V. Mlýnský, M. Janeček, P. Kührová, M. Krepl, P. Banás*, J. Šponer, and **G. Bussi***
Automatic Learning of Hydrogen-Bond Fixes in the AMBER RNA Force Field
J. Chem. Theory Comput. 18, 4490 (2022)
Preprint: arXiv:2201.04078

21. V. Mlýnský*, M. Janeček, P. Kührová, T. Fröhlking, M. Otyepka, **G. Bussi**, P. Banás*, J. Šponer*
Toward Convergence in Folding Simulations of RNA Tetraloops: Comparison of Enhanced Sampling Techniques and Effects of Force Field Corrections
J. Chem. Theory Comput. 18, 2642 (2022)
Preprint: bioRxiv doi:10.1101/2021.11.30.470631

22. V. Del Tatto, P. Raiteri, M. Bernetti, and **G. Bussi***
Molecular dynamics of solids at constant pressure and stress using anisotropic stochastic cell rescaling
Appl. Sci. 12, 1139 (2022)

23. M. Bernetti* and **G. Bussi***
Comparing state-of-the-art approaches to back-calculate SAXS spectra from atomistic molecular dynamics simulations
Eur. Phys. J. B 94, 180 (2021)

24. M. Paloni, **G. Bussi**, and A. Barducci*
Arginine multivalency stabilizes protein/RNA condensates
Protein Sci. 30, 1418 (2021)
Preprint: bioRxiv doi:10.1101/2021.04.22.440959

25. M. Bernetti*, K. B. Hall, and **G. Bussi***
Reweighting of molecular simulations with explicit-solvent SAXS restraints elucidates ion-dependent RNA ensembles
Nucleic Acids Res. 49, e84 (2021)
Preprint: arXiv:2103.04964

26. S. Bottaro*, **G. Bussi**, and K. Lindorf-Larssen*
Conformational Ensembles of Non-Coding Elements in the SARS-CoV-2 Genome from Molecular Dynamics Simulations
J. Am. Chem. Soc. 143, 8333 (2021)
Preprint: bioRxiv doi:10.1101/2020.12.11.421784

27. N. Calonaci, A. Jones, F. Cuturello, M. Sattler, and **G. Bussi***
Machine learning a model for RNA structure prediction
NAR Genom. Bioinform. 2, lqaa090 (2020)
Preprint: arXiv:2004.00351

28. M. Bernetti and **G. Bussi***
Pressure control using stochastic cell rescaling
J. Chem. Phys. 153, 114107 (2020)
Preprint: arXiv:2006.09250

29. A. Suma, L. Coronel, **G. Bussi**, and C. Micheletti*
Directional translocation resistance of Zika xrRNA
Nat. Commun. 11, 3749 (2020)
Preprint: bioRxiv doi:10.1101/2020.06.17.157297

30. T. Fröhlking, M. Bernetti, N. Calonaci, and **G. Bussi***
Toward empirical force fields that match experimental observables
J. Chem. Phys. 152, 230902 (2020)
Preprint: arXiv:2004.01630

31. V. Mlýnský*, P. Kührová, T. Kühr, M. Otyepka, **G. Bussi**, P. Banás, and J. Šponer*
Fine-tuning of the AMBER RNA Force Field with a New Term Adjusting Interactions of Terminal Nucleotides
J. Chem. Theory Comput. 16, 3936 (2020)
Preprint: bioRxiv doi:10.1101/2020.03.08.982538

32. F. Cuturello, G. Tiana, and **G. Bussi***
Assessing the accuracy of direct-coupling analysis for RNA contact prediction
RNA 26, 637 (2020)
Preprint: arXiv:1812.07630

33. **G. Bussi** and A. Laio*
Using metadynamics to explore complex free-energy landscapes
Nat. Rev. Phys. 2, 200 (2020)

34. S. Reißer*, S. Zucchelli, S. Gustincich, and **G. Bussi***
Conformational ensembles of an RNA hairpin using molecular dynamics and sparse NMR data,
Nucleic Acids Res. 48, 1164 (2020)

35. F. Colizzi*, C. Perez-Gonzalez, R. Fritzen, Y. Levy, M. F. White, J. C. Penedo*, and **G. Bussi***
Asymmetric base-pair opening drives helicase unwinding dynamics
Proc. Natl. Acad. Sci. U.S.A. 116, 22471 (2019)

36. M. Bonomi*, **G. Bussi***, C. Camilloni*, G. Tribello*, et al
A community effort to promote transparency and reproducibility in enhanced molecular simulations.
Nat. Methods 16, 670 (2019)

37. A. Cesari, S. Bottaro, K. Lindorff-Larsen, P. Banás, J. Šponer, and **G. Bussi***
Fitting corrections to an RNA force field using experimental data
J. Chem. Theory Comput. 15, 3425 (2019)

38. G. Franco, M. Cagiada, **G. Bussi**, and G. Tiana*
Statistical mechanical properties of sequence space determine the efficiency of the various algorithms to predict interaction energies and native contacts from protein coevolution
Phys. Biol. 16, 046007 (2019)
Preprint: arXiv:1902.01155

39. G. Pinamonti*, F. Paul, F. Noé, A. Rodrigues, and **G. Bussi***
The mechanism of RNA base fraying: molecular dynamics simulations analyzed with

core-set Markov state models.
J. Chem. Phys. 150, 154123 (2019)
Preprint: arXiv:1811.12144

40. P. Kührová, V. Mlýnský, M. Zgarbová, M. Krepl, **G. Bussi**, R. B. Best, M. Otyepka, J. Šponer*, and P. Banáš*
Improving the performance of the RNA AMBER force field by tuning the hydrogen-bonding interactions
J. Chem. Theory Comput. 15, 3288 (2019)
Preprint: bioRxiv doi:10.1101/410993

41. S. Bottaro*, **G. Bussi***, G. Pinamonti, S. Reißer, W. Boomsma, and K. Lindorff-Larsen
Barnaba: Software for Analysis of Nucleic Acids Structures and Trajectories.
RNA 25, 219 (2019)
Preprint: bioRxiv doi:10.1101/345678

42. R. Rangan, M. Bonomi*, G. Heller, A. Cesari, **G. Bussi**, and M. Vendruscolo*
Determination of Structural Ensembles of Proteins: Restraining vs Reweighting.
J. Chem. Theory Comput. 14, 6632 (2018)

43. N. Hildebrand, M. Michaelis, N. Wurzler, Z. Li, J. D. Hirst, A. Micsonai, J. Kardos, A. Gil-Ley, **G. Bussi**, S. Köppen, M. Delle Piane*, and L. Colombi Ciacchi
Atomistic Details of Chymotrypsin Conformational Changes upon Adsorption on Silica.
ACS Biomater. Sci. Eng. 4, 4036 (2018)

44. S. Bottaro*, **G. Bussi**, S. D. Kennedy, D. H. Turner, and K. Lindorff-Larsen*
Conformational ensembles of RNA oligonucleotides from integrating NMR and molecular simulations
Sci. Adv. 4, eaar8521 (2018)
Preprint: bioRxiv doi:10.1101/230268

45. J. Šponer*, **G. Bussi***, M. Krepl, P. Banáš, S. Bottaro, R. A. Cunha, A. Gil-Ley, G. Pinamonti, S. Poblete, P. Jurečka, N. G. Walter, and M. Otyepka
RNA Structural Dynamics as Captured by Molecular Simulations: A Comprehensive Overview
Chem. Rev. 118, 4177 (2018)

46. S. Poblete*, S. Bottaro, and **G. Bussi**
Effects and limitations of a nucleobase-driven backmapping procedure for nucleic acids using steered Molecular Dynamics,
Biochem. Biophys. Res. Commun. 498, 352 (2018)
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51. V. Mlýnský* and **G. Bussi***
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Preprint: arXiv:1612.05882

54. V. Mlýnský* and **G. Bussi***
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Nucleic Acids Res. 42, 13306 (2014)
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AIP Conf. Proc. 772, 1025 (2005)

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112. A. Ruini*, **G. Bussi**, A. Ferretti, M. J. Caldas, and E. Molinari,
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Book chapters

1. V. Piomponi, M. Bernetti, and **G. Bussi***
   Molecular dynamics simulations of chemically modified ribonucleotides
   in *RNA Structure and Function*, edited by J. Barciszewski
   RNA Technologies, 14 (2023)
   Preprint: arXiv:2211.13657

2. **G. Bussi**, A. Laio*, and P. Tiwary
   Metadynamics: a unified framework for accelerating rare events and sampling thermodynamics and kinetics
   in *Handbook of Materials Modeling. Volume 1 Methods: Theory and Modeling*, edited by W. Andreoni and S. Yip
   Handbook of Materials Modeling, 565 (2020)

3. **G. Bussi*** and G. A. Tribello*
   Analyzing and biasing simulations with PLUMED
   in *Biomolecular Simulations: Methods and Protocols*, edited by M. Bonomi and C. Camilloni
   Methods Mol. Biol. 2022, 529 (2019)
   Preprint: arXiv:1812.08213

4. F. Di Palma, F. Colizzi, and **G. Bussi***
   Using reweighted pulling simulations to characterize conformational changes in riboswitches
   in *Computational Methods for Understanding Riboswitches*
   Meth. Enzymol. 553, 139 (2015)

5. **G. Bussi** and D. Branduardi
   Free-energy Calculations with Metadynamics: Theory and Practice,
   Rev. Comp. Chem. 27, 1 (2015)

6. F. Colizzi, A. M. Lamontagne, D. A. Lafontaine, and **G. Bussi**
   Probing Riboswitch Binding Sites with Molecular Docking, Focused Libraries, and In-line Probing Assays,
   in *Therapeutic Applications of Ribozymes and Riboswitches*, edited by D. A. Lafontaine and A. Dubé
   Methods Mol. Biol. 1103, 141 (2014)

7. **G. Bussi**, F. L. Gervasio, A. Laio and M. Parrinello,
   Protein folding with combined parallel tempering and metadynamics,
   in *HPC-Europa: Science and Supercomputing in Europe* (2006), edited by P. Alberigo, G. Erbacci and F. Garofalo.

8. **G. Bussi**, A. Ferretti, A. Ruini, M. J. Caldas, and E. Molinari,
   Optics and transport in conjugated polymer crystals: interchain interaction effects,
   Adv. Solid State Phys. 43, 313 (2003)

9. A. Ruini, M. J. Caldas, **G. Bussi**, A. Ferretti, B. M. Silva, G. Goldoni, and E. Molinari,
   Optical properties of organic materials: from single molecules to solid state,
   in *Radiation-Matter Interaction in Confined Systems*, edited by L. C. Andreani, G. Benedek, and E. Molinari (Società Italiana di Fisica, Bologna, 2002).

Oral presentations at conferences and seminars

- November 29–December 2, 2022: Workshop on advanced biomolecule modeling techniques, UNAM, Mexico City, Mexico.
  Invited talk: *Combining atomistic molecular dynamics simulations and solution experiments to investigate RNA dynamics*.
- October 13–14, 2022: 2nd Disva-Masbic Annual Symposium: Protein Structure and Function in Biology, Medicine and Nanotechnology, Ancona, Italy.
  Invited talk: *Combining atomistic molecular dynamics simulations and solution experiments to investigate RNA dynamics*.
- October 10–11, 2022: CECAM workshop on Electronic Structure Software Development: Best Practices and Tools Lausanne, Switzerland.
  Invited talk: *Developing and maintaining PLUMED, a plugin for classical and ab initio molecular dynamics*.
- June 06–08, 2022: 8th Annual CCPBioSim Conference - Frontiers in Biomolecular Simulation 2022.
  Invited talk: *Learning RNA force fields from experimental data*.
- December 13–17, 2021: 3rd Conference on Biomotors, Virus Assembly, and RNA Nanobiotechnology, virtual conference.
  Invited talk: *RNA structural dynamics combining solution experiments and molecular simulations*.
- November 23–26, 2021: CECAM workshop on "Co-evolutionary analysis meets machine learning for modelling biomolecular structures and interactions", Lausanne, Switzerland.
  Invited talk: *Using machine learning to improve RNA structure prediction*.
- July 13–17, 2021: Telluride workshop on RNA Dynamics, Telluride, U.S.A. (virtual participation)
  Invited talk: *RNA structural dynamics combining molecular dynamics and solution experiments*.
- February 5–8, 2020: Physics of Biomolecules: Structure, Dynamics, and Function, Bressanone, Italy,
  Invited talk: *Probing RNA dynamics with molecular simulations and solution experiments*.
- July 8–11, 2019: Telluride workshop on RNA Dynamics, Telluride, U.S.A.
  Invited talk: *RNA dynamics: Combining molecular dynamics & solution experiments*.
- June 5–July 7, 2019: Mainz Materials Simulation Days 2019, Mainz, Germany.
  Invited talk: *Using enhanced sampling simulations to characterize RNA structural dynamics*.
- March 14–15, 2019: Molecular Dynamics Today, University of Bologna, Italy.
  Invited talk: *Using molecular simulations to characterize RNA dynamics*.
- December 13, 2018: IRB Barcelona, Spain.
  Seminar: *Using molecular simulations and solution experiments to predict RNA structural dynamics and refine empirical force fields*.

- October 16–18, 2018: Norwegian National Meeting in Chemistry, Lillestrøm, Norway.
  Invited talk: *RNA structure and dynamics combining molecular simulations and experiments*.

- September 3–6, 2018: CECAM workshop on "Computational biophysics on your desktop: is that possible?", University of Trento, Italy.
  Invited talk: *RNA structure and dynamics using models at different resolution and experimental data*.

- June 26–30, 2018: Telluride workshop on Challenges in RNA Structural Modeling and Design, Telluride, U.S.A.
  Invited talk: *Modeling RNA structural dynamics using molecular simulations and experimental data*.

- June 25, 2018: Center for Non Linear Sciences, Los Alamos, U.S.A.
  Seminar: *Using molecular simulations and solution experiments to predict RNA structural dynamics*.

- May 23–25, 2018: CECAM workshop on "Building the bridge between theories and software: SME as a boost for technology transfer in industrial simulative pipelines" IIT, Genova, Italy.
  Invited talk: *Using molecular dynamics simulations to study interaction of RNA with small molecules*.

- May 15–20, 2018: Erice School: Exploring and Quantifying Rough Free Energy Landscapes, Erice, Italy,
  Invited talk: *Combining molecular simulations and solution experiments to characterize RNA structural dynamics*.

- April 23, 2018: Department of Chemistry, Technische Universität München, Germany,
  Seminar: *Using molecular simulations and solution experiments to predict RNA structural dynamics*.

- March 15, 2018: Condensed Matter Physics, University of Barcelona, Spain,
  Seminar: *Using molecular simulations to predict and explain RNA structural dynamics*.

- February 7–10, 2018: Physics of Biomolecules: Structure, Dynamics, and Function, Bressanone, Italy,
  Invited talk: *Using molecular dynamics simulations to study interaction of RNA with small molecules*.

- January 18, 2018: Department of Biology, University of Copenhagen, Denmark,
  Seminar: *Using molecular simulations and solution experiments to predict RNA structural dynamics*.

- December 5–6, 2017: ENS de Lyon meets SISSA, Lyon, France,
  Invited talk: *Using molecular simulations and NMR experiments to predict RNA structural dynamics*.

- November 24, 2017: Department of Physics, University of Milano, Italy,
  Seminar: *Using molecular dynamics simulations to study interaction of RNA with small molecules*.

- September 19, 2017: Department of Physics, University of Milano, Italy,
  Seminar: *RNA structure and dynamics: combining molecular dynamics, solution experiments, and coevolutionary information.*
- July 24–28, 2017: Telluride workshop on RNA Dynamics, Telluride, U.S.A.
  Invited talk: *RNA dynamics: Combining molecular dynamics & solution experiments.*
- November 28, 2016: Department of Chemistry, University of Innsbruck, Austria,
  Seminar: *RNA dynamics: insights from molecular dynamics simulations.*
- October 7–12, 2016: Erice School: Exploring and Quantifying Rough Free Energy Landscapes, Erice, Italy,
  Invited talk: *Sampling the conformational landscape of oligonucleotides using molecular dynamics.*
- September 28, 2016: Laboratory of Molecular Function and Design, Strasbourg, France,
  Seminar: *RNA dynamics: insights from molecular dynamics simulations.*
- August 31, 2016: Chemistry Department, University of Vienna, Austria,
  Seminar: *Molecular dynamics simulations of RNA oligonucleotides.*
- May 24–27, 2016: Organizer of a workshop on RNA structures, dynamics, and function, SISSA, Trieste, Italy,
  Invited talk: *Interaction of RNA with Mg and SHAPE reagents and A coarse-grained model for structure prediction.*
- February 3–6, 2016: Physics of Biomolecules: Structure, Dynamics, and Function, Bressanone, Italy,
  Invited talk: *RNA dynamics: what we can learn from molecular simulations.*
- November 30, 2015: RNA structure and function – computational and experimental approaches Minisymposium, Warsaw, Poland.
  Invited talk: *Computational approaches to RNA: from atomistic molecular dynamics to structural bioinformatics.*
- September 28–October 2, 2015: Italian National Conference on Condensed Matter Physics FISMAT2015, Palermo, Italy.
  Invited talk: *Computational approaches to RNA unzipping dynamics.*
- September 16–18, 2015: CECAM workshop "From trajectories to reaction coordinates: making sense of molecular simulation data" Vienna, Austria.
  Invited talk: *RNA dynamics in stop motion: from crystal structures to trajectories.*
- July 20–24, 2015: Telluride workshop on RNA Dynamics, Telluride, U.S.A.
  Invited talk: *RNA dynamics: learning from molecular dynamics and analysis of X-ray structures.*
- June 5–6, 2015: Collaborative workshop on RNA: structure, function and evolution, SISSA, Trieste, Italy.
  Invited talk: *RNA and ions: learning from atomistic molecular dynamics.*

- May 26–31, 2015: RNA society meeting, Madison, U.S.A.
  Contributed talk: *Conformational changes in the adenine riboswitch using molecular dynamics and enhanced sampling techniques: understanding the role of ligand and Mg2+.*

- March 9–11, 2015: Workshop "Computing Free-Energy Across Disciplines," Münster, Germany.
  Invited talk: *Using free-energy methods to study RNA conformational transitions.*

- January 22, 2015: Center for Theoretical Biological Physics of Rice University, Houston, U.S.A.
  Seminar: *RNAs in silico: what we can learn from molecular dynamics.*

- November 20–21, 2014: CECAM workshop on "Advanced Modeling to Investigate Biomolecules" IIT, Genova, Italy.
  Invited talk: *The Role of Nucleobase Interactions in RNA Structure and Dynamics.*

- September 8, 2014: Institut de Biologie Physico-Chimique, Paris France.
  Seminar: *RNAs in silico: what we can learn from molecular dynamics.*

- September 1–6, 2014: Meeting on "Biological applications of metadynamics", organized by Prof. Michele Parrinello, Castasegna, Switzerland.
  Invited talk: *A metadynamics way to Hamiltonian replica exchange.*

- June 10–12, 2014: CECAM workshop on "Binding free energy and kinetics: computation meets experiments" IIT, Genova, Italy.
  Invited talk: *RNAs in Silico: What we can Learn from Enhanced Molecular Dynamics.*

- June 3–8, 2014: RNA society meeting, Quebec City, Canada.
  Contributed talk: *Nearest neighbor parameters for RNA from accurate atomistic simulations.*

- April 23, 2014: Olomuc University, Czech Republic.
  Seminar: *Enhanced sampling for RNA conformational transitions.*

- March 27, 2014: IMP, Vienna, Austria.
  Seminar: *RNAs in silico: what we can learn from molecular dynamics.*

- March 11, 2014: Università della Svizzera Italiana, Lugano, Switzerland.
  Seminar: *A metadynamics way to Hamiltonian replica exchange.*

- February 6–8, 2014: Workshop on Protein Physics: Structure, Dynamics, and Function, Bressanone, Italy,
  Invited talk: *RNAs in silico: learning from molecular dynamics and enhanced sampling techniques.*

- October 28, 2013: Università Federico II, Napoli, Italy
  Seminar: *RNAs in silico: learning from molecular dynamics and enhanced sampling techniques.*

- September 2–6, 2013: CPMD 2013, Leipzig, Germany.
  Invited talk: *RNAs in silico: learning from molecular dynamics and enhanced sampling techniques.*

- April 7–11, 2013: American Chemical Society 245th National Meeting & Exposition, New Orleans, USA.
  Contributed talk: *Conformational transitions in adenine sensing riboswitch: A computational study*.
  Contributed talk: *Metadynamics with adaptive Gaussians*.

- February 20, 2013: GeorgiaTech, Atlanta, USA
  Seminar: *RNAs in silico: what can we learn from accelerated molecular simulations*.

- February 17–22, 2013: 53rd Sanibel Symposium, St. Simons Island, Georgia, USA
  Invited talk: *RNAs in silico: what we can learn from metadynamics and steered molecular dynamics*.

- February 4–6, 2013: Computationally Driven Drug Discovery meeting, IIT, Genova, Italy
  Contributed talk: *Exploiting electrostatics in RNA/peptide binding*.

- August 6–10, 2012: ICERM Workshop "Bridging Scales in Computational Polymer Chemistry," Providence, USA
  Invited talk: *Accelerated sampling of the conformational space in biopolymers: from small proteins to RNA*.

- July 27, 2012: Dept. of Bioengineering and Therapeutic Sciences, University of California, San Francisco, USA
  Seminar: *RNAs in silico: what we can learn from accelerated molecular simulations*.

- July 24, 2012: QB3 Institute, Berkeley, USA
  Seminar: *RNAs in silico: what we can learn from accelerated molecular simulations*.

- June 19–20, 2012: Organizer of the "First PLUMED meeting" held in SISSA, Trieste.

- February 16–18, 2012: Second Workshop on Physics of Protein Folding and Aggregation, Bressanone, Italy,
  Invited talk: *Accelerated sampling of the conformational space in biomolecules: from small proteins to RNA*.

- January 27, 2012: Ludwig-Maximilians-Universität München, Germany
  Seminar: *Sampling the conformational space in biomolecules: from small proteins to RNA*.

- September 5–9, 2011: CPMD 2011, Barcelona, Spain
  Invited talk: *Accelerated sampling of the conformational space in biomolecules: from small proteins to RNA*.

- July 7–8, 2011: Topical Meeting on Structural Bioinformatics and Computational Biophysics SISSA, Trieste, Italy.
  Invited talk: *Accelerated sampling of the conformational space in biomolecules: from small proteins to RNA*.

- April 19, 2011: German Research School for Simulation Sciences, Germany
  Seminar: *Accelerated sampling of the conformational space in biomolecules: from small proteins to RNA*.

- April 8, 2011: Bremen Center for Computational Material Science, Germany
  Seminar: *New approaches in molecular dynamics: from stochastic thermostats to rare-event sampling*.
- February 7, 2011: Università della Svizzera Italiana, Lugano, Switzerland.
  Seminar: *Enhanced sampling for small RNAs*.
- January 13–15, 2011: 15th International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods, ICTP, Trieste, Italy.
  Invited talk: *Stochastic thermostats in classical and ab initio molecular dynamics*.
- December 1, 2010: Department of Chemistry, University of Cambridge, UK
  Seminar: *New approaches in molecular dynamics: from stochastic thermostats to rare-event sampling*.
- June 6–9, 2010: CECAM workshop on Advances in the Implementation of Polarizable Force Fields for Molecular Simulations, Lausanne, Switzerland.
  Contributed talk: *A colored noise thermostat for Car-Parrinello/polarizable force fields*.
- February 11–12, 2010: Workshop on Physics of Protein Folding and Aggregation, Bressanone, Italy,
  Invited talk: *Folding proteins in explicit solvent with parallel tempering metadynamics simulations*.
- February 1–5, 2010: First International Workshop on Computational Biophysics (IWCBP-1), Ho Chi Minh City, Vietnam,
  Invited talk: *Stochastic thermostats in classical and ab initio molecular dynamics*.
- September 29–October 4, 2009: International Conference of Computational Methods in Sciences and Engineering, Rhodes, Greece,
  Invited talk: *Folding proteins with explicit solvent molecular dynamics simulations*.
- July 27–29, 2009: CECAM workshop on Fundamental aspects of deterministic thermostats, Lausanne, Switzerland.
  Invited talk: *Stochastic thermostats in classical and ab initio molecular dynamics*.
- March 3, 2009: Chemistry Department, UC Davis, USA.
  Seminar: *New approaches in molecular dynamics: from stochastic thermostats to rare-event sampling*.
- February 23–27, 2009: IPAM workshop on Rare Events in high dimensional systems, UCLA, Los Angeles, USA,
  Invited talk: *Rare events: landscapes and diffusion with metadynamics and maximum likelihood*.
- December 2, 2008: Physics Department, King's College London, UK,
  Seminar: *Simulation of (bio)molecules: from equilibrium to nonequilibrium processes*.
- November 18, 2008: Physics Department, Mainz Universitat, Germany.
  Seminar: *New approaches in molecular dynamics: from stochastic thermostats to rare-event sampling*.

- October 31, 2008: Physics Department, King's College London, UK,
  Seminar: *Stochastic thermostats in classical and ab initio molecular dynamics*.
- June 23–27, 2008: CPMD 2008, ICTP, Trieste, Italy
  Invited talk: *Stochastic thermostats in classical and ab initio molecular dynamics*.
- May 27–31, 2008: Calcolo Scientifico nella Fisica Italiana - CSFI 2008, Rimini, Italy.
  Invited talk: *Free energy landscapes with metadynamics and parallel tempering*.
- April 15, 2008: ICTP, Trieste, Italy
  Seminar: *New approaches in molecular dynamics: from stochastic thermostats to rare-event sampling*.
- April 11, 2008: SISSA, Trieste, Italy
  Seminar: *Simulation of (bio)molecules: from equilibrium to nonequilibrium processes*.
- March 10–14, 2008: March Meeting, American Physical Society, New Orleans, USA.
  Contributed talk: *Well-tempered metadynamics: a smoothly-converging and tunable free energy method*.
  Contributed talk: *Canonical sampling through velocity rescaling*.
- February 18–22, 2008: Metastability and Rare Events in Complex Systems, Vienna, Austria.
  Contributed talk: *Well-tempered metadynamics: a smoothly-converging and tunable free energy method*.
- September 5–8, 2007: CCP2007, Conference on Computational Physics, Brussels, Belgium.
  Contributed talk: *Canonical sampling through velocity rescaling*.
- August 19–23, 2007: American Chemical Society 234th National Meeting & Exposition Boston, USA.
  Contributed talk: *Free-energy landscapes from combined parallel-tempering and metadynamics*.
  Contributed talk: *Canonical sampling through velocity rescaling*.
- April 25, 2007: Physics Department, King's College London,UK, in collaboration with F. L. Gervasio.
  Seminar: *Accurate free energies and reactive paths of biologically relevant events from atomistic simulations*.
- April 2–4, 2007: Progress in *ab initio* modeling of biomolecules: towards computational spectroscopy, Rome, Italy.
  Invited talk: *Beta-hairpin folding with parallel tempering and metadynamics*.
- July 17, 2006: National Center of CNR-INFM S3, Modena, Italy.
  Seminar: *Free energy landscapes from combined metadynamics and parallel tempering: from model systems to protein folding*.
- July 3–7, 2006: Progress in *ab initio* modeling of biomolecules: methods and applications, Lorentz Center, Leiden Netherlands.
  Invited talk: *Free energy landscapes from combined metadynamics and parallel tempering*.

- November 15–16, 2005: NANOQUANTA mini-workshop: "Specification of file formats for NANOQUANTA", Louvain-la-Neuve, Belgium.
  Invited talk: *Ideas about file formats*.
- July 26–30, 2004: 27th International Conference on the Physics of Semiconductors, Flagstaff, Arizona, USA.
  Contributed talk: *Excitons in carbon nanotubes: a first-principles study*.
- May 7, 2004: Università della Svizzera Italiana, Lugano, Switzerland.
  Seminar: *Optical excitations of polymers and carbon nanotubes from first-principles*.
- April 13–15, 2004: EXC!TiNG Network Meeting 3, Aarhus, Denmark.
  Contributed talk: *Excitons in carbon nanotubes: a first-principles study*.
- February 25–27, 2004: 2nd National Conference on Nanoscience and Nanotechnology: The Molecular Approach, Bologna, Italy.
  Contributed talk: *Excitons in carbon nanotubes: a first-principles study*.
- April 14–16, 2003: EXC!TiNG Network Meeting 2, Louvain, Belgium.
  Contributed talk: *Optics and transport in conjugated polymer crystals: interchain interaction effects*.
- June 24–28, 2002: INFMeeting 2002, Bari, Italy.
  Contributed talk: *First principles study of optical properties in semiconducting conjugated polymers: interchain effects and Davydov splitting*.

Other interests

- Music, especially jazz.
- Playing piano and keyboards.