Dr. Rafael C. Bernardi

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Beckman Institute for Advanced Science and Technology
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Education

2010 **Ph.D. Biophysics, Federal University of Rio de Janeiro, Brazil – (advisor: P.G. Pascutti)**

***** PhD Internship (Brazilian "Sandwich" PhD Fellowship Program) – University of Pennsylvania** – Klein's lab (Fall, 2008)

2007 **M.Sc. Physics, Brazilian Center for Physical Research, Brazil – (advisor: C.A. Taft)**

2005 **B.Sc. Physics, State University of Londrina, Brazil – (advisor: A.T. Ota)**

Research Experience

2017- **Research Scientist – University of Illinois**

2017-2017 **Visiting Professor of Applied Physics – LMU, Munich – Germany**

2012-2017 **Postdoctoral Research Associate – University of Illinois**

2010-2012 **Researcher at Laboratory of Biotechnology – INMETRO, Brazil**

Honors and Recognitions

2010 **Best PhD Thesis** in 2010 in the field of Biophysics and Biotechnology – *Casimiro Montenegro Filho National Award* – Bureau of Strategic Affair of the Brazilian Presidency, 2010.

Most Relevant Publications (see full list at the end of this document)

1. LF Milles, K Schulten, HE Gaub‡, RC Bernardi‡; *Molecular mechanism of extreme mechanostability in a pathogen surface anchor*; **Science**, 359 (6383), 1527-1533, **2018**
2. MCR Melo*, RC Bernardi*, T Rudack, M Scheurer, C Riplinger, JC Phillips, JDC Maia, GB Rocha, JV Ribeiro, JE Stone, F Neese, K Schulten, Z Luthey-Schulten; *NAMD goes quantum: A new integrative suite for hybrid simulations*; **Nature Methods**, 15 (5), 351-354, **2018**
3. RC Bernardi‡*, E Durner*, C Schoeler, KH Malinowska, BG Carvalho, EA Bayer, Z Luthey-Schulten, HE Gaub, MA Nash‡; *Mechanisms of Nanonewton Mechanostability in a Protein Complex Revealed by Molecular Dynamics Simulations and Single-Molecule Force Spectroscopy*; **Journal of the American Chemical Society**, 141 (37), 14752-14763, **2019**
4. C Schoeler*, RC Bernardi*, KH Malinowska, E Durner, W Ott; EA Bayer; K Schulten; MA Nash; HE Gaub; *Mapping mechanical force propagation through biomolecular complexes*; **Nano Letters**, 15 (11), 7370-7376, **2015** – *Cover Article*
5. SM Sedlak*, LC Schendel*, MCR Melo, DA Pippig, Z Luthey-Schulten, HE Gaub, RC Bernardi‡; *Direction Matters – Monovalent Streptavidin/Biotin Complex under Load*; **Nano Letters**, 19 (6), 3415-3421, **2019** – *Cover Article*

* **Co-first author (equally contributing)**

‡ **Corresponding Author**

Cover Articles

Jun 2019 – Nano Letters

Direction Matters – Monovalent Streptavidin/Biotin Complex under Load; *SM Sedlak, LC Schendel, MCR Melo, DA Pippig, Z Luthey-Schulten, HE Gaub, RC Bernardi*

Feb 2018 – Biophysical Journal

PyContact: Rapid, Customizable and Visual Analysis ofNon-Covalent Interactions in MD Simulations; *M Scheurer, P Rodenkirch, M Siggel, RC Bernardi, K Schulten, E Tajkhorshid, T Rudack*

Dec 2017 – Journal of The American Chemical Society

Combining in Vitro and in Silico Single Molecule Force Spectroscopy to Characterize and Tune Cellulosomal Scaffoldin Mechanics; *T Verdorfer, RC Bernardi, A Meinhold, W Ott, Z Luthey-Schulten, MA Nash, HE Gaub*

Nov 2015 – Nano Letters

Mapping mechanical force propagation through biomolecular complexes; *C Schoeler*; RC Bernardi*; KH Malinowska; E Durner; W Ott; EA Bayer; K Schulten; MA Nash; HE Gaub*

Selected Media Coverage of Publications

Sep 2019 – Journal of the American Chemical Society

(Altmetric Score 12 – High Attention Score comparted to articles of same age – 84 percentile)

1. University of Illinois Website (frontpage) – *Computational models used to predict behavior of protein complexes*.
2. Nanowerk – *Computational models used to predict behavior of protein complexes*.

Jan 2019 – Structure

(Altmetric Score 48 – High Attention Score comparted to articles of same age – 94 percentile)

1. EurekAlert! – *Impaired cellular force transmission a cause for valvular heart disease*.
2. The Medical News – *Researchers shed light on molecular mechanisms of heart valvular disease*.
3. Technology Networks – *Impaired transmission of cellular force - culprit in valvular heart disease.*
4. Medinida – *Cause for valvular heart disease discovered.*

May 2018 – Nature Methods

(Altmetric Score 94 – High Attention Score comparted to articles of same age – 97 percentile)

1. University of Illinois Website (frontpage) –*Team brings subatomic resolution to computational microscope*.
2. EurekAlert! – *Team brings subatomic resolution to computational microscope*.
3. Primeur Magazine – *University of Illinois team brings subatomic resolution to computational microscope*.
4. NSF Science360 News – *Team brings subatomic resolution to computational microscope*.

Mar 2018 – Science

(Altmetric Score 115 – High Attention Score comparted to articles of same age – 98 percentile)

1. Science – *How a pathogen holds on to its host*.
2. Cell – *Leading Edge Select: Breaking the rules.*
3. HPC Wire – *Blue Waters reveals how staph bacteria cling to human cells*.
4. Nanowerk – *An alternative to antibiotics - wakening superbugs' grip*.
5. Science Newsline – *Biophysics: Bacterial adhesion in vitro and in silico*.
6. Technology.org – *Night of the living bacteria: how GPUs aid fight against zombie-like bugs*.

Nov 2015 – Nano Letters

(Altmetric Score 20 – High Attention Score comparted to articles of same age – 92 percentile)

1. Physics World – *Protein pulling reveals a new way that molecules resist external forces*.
2. Scientific Computing – *Cellulosomes: One of life's strongest biomolecular bonds discovered with use of supercomputers*.

Dec 2014 – Nature Communications

(Altmetric Score 42 – High Attention Score comparted to articles of same age – 96 percentile)

1. Phys.org – *Supercomputers help solve puzzle-like bond for biofuels*.
2. Scientific Computing – *Solving puzzle-like bond for biofuels: first look at one of nature's strongest biomolecular interactions*.
3. NSF Science 360 News (Video) – *Jordan and Charlie delve into life's strongest bond*.

Recent Invited Talks

2020 – Mar **ACS National Meeting & Expo**, Philadelphia, PA, USA – upcoming

2019 – Nov **XX Brazilian Symposium on Theoretical Chemistry**, João Pessoa, Brazil

2019 – Nov **Carlos Chagas Institute of Biophysics**, Federal University of Rio de Janeiro, Brazil

2019 – Jul **Congress of the International Society for Theoretical Chemical Physics**, Tromsø, Norway

2019 – Jan **Center for Theoretical Biological Physics**, Rice University, Houston, TX, USA

2019 – Jan **Department of Chemistry**, University of Illinois at Urbana-Champaign, IL, USA

2019 – Jan **Beckman Institute**, University of Illinois at Urbana-Champaign, IL, USA

2018 – Nov **NSF Workshop: Quantum Biology and Quantum Processes in Biology**, Tysons Corner, VA, USA

2018 – Oct **Department of Physics Colloquium**, University of Wisconsin Milwaukee, WI, USA

2018 – Aug **Key Challenges in Biophysics**, Kloster Seeon, Germany

2018 – Jun **Blue Waters Symposium**, Sunriver, OR, USA

2018 – Mar **255th ACS National Meeting**, New Orleans, LA, USA

2017 – Nov **Joint Colloquium of CeNS and the Department of Physics**, Center for NanoScience, Ludwig-Maximilians-Universität München, Germany

2017 – Oct **Klaus Schulten Memorial Symposium** – Munich, Germany

2017 – Jul **Gordon Research Conference** – Cellulases & Other Carbohydrate-Active Enzymes, Andover (NH), USA

2017 – Mar **Department of Biophysics and Molecular Materials**, Ludwig-Maximilians-Universität München, Germany

2016 – Sep **Department of Biophysics and Molecular Materials**, Ludwig-Maximilians-Universität München, Germany

2016 – Jun **Blue Waters Symposium**, Sunriver, OR, USA

2016 – Mar **American Physical Society Meeting 2016**, Statistical Analysis and Molecular Dynamics Simulations of Biological Systems, Baltimore, USA

2015 – Oct **Department of Biophysics and Molecular Materials**, Ludwig-Maximilians-Universität München, Germany

2014 – Nov **Second Generation Bioethanol 2014**, Brazilian Bioethanol Science and Technology Laboratory, Brazil

2014 – Mar **Department of Biophysics and Molecular Materials**, Ludwig-Maximilians-Universität München, Germany

2013 – Oct **Energy Biosciences Institute Seminar**, University of California – Berkeley, USA

Recent Teaching Experience

2019 **Workshop Instructor:** Center for the Physics of Living Cells Summer School, University of Illinois at Urbana-Champaign, Urbana

2019 **Workshop Instructor:** NSF-sponsored Summer Research Experience for Undergraduates (REU) Program, University of Illinois at Urbana-Champaign, Urbana

2018 **Guest Lecture:** NAMD and VMD combined for easy and fast QM/MM simulations, School of Molecular Modeling applied to Biological Systems, National Laboratory of Scientific Computation, Petropolis, Brazil

2018 **Guest Lecture:** Bridging the gap between *in silico* and *in vitro* force spectroscopy, School of Molecular Modeling applied to Biological Systems, National Laboratory of Scientific Computation, Petropolis, Brazil

2018 **Laboratory Instructor:** Quantum Methods of QM/MM, School of Molecular Modeling applied to Biological Systems, National Laboratory of Scientific Computation, Petropolis, Brazil

2018 **Workshop Instructor:** Hands-On Workshop on QM/MM Simulations, University of Illinois at Urbana-Champaign, Urbana

2017 **Workshop Instructor:** NSF Center for the Physics of Living Cells Summer School 2017, University of Illinois at Urbana-Champaign, Urbana

2016 **Workshop Instructor:** Hands-On Workshop on Integrative Modeling and Simulations, University of California, San Francisco

2016 **Workshop Instructor:** Hands-On Workshop on Computational Biophysics, Georgia Institute of Technology, Atlanta

2016 **Workshop Instructor:** Hands-On Workshop on Computational Biophysics, University of Illinois at Urbana-Champaign, Urbana

2016 **Workshop Instructor:** Hands-On Workshop on Cryo-EM Guided Modeling and Simulation, Jülich Supercomputing Centre, Jülich, Germany

2015 **Workshop Teaching Assistant:** Hands-On Workshop on Computational Biophysics, University of Southern Denmark, Odense, Denmark

2014 **Laboratory Instructor:** Molecular Dynamics Simulations, School of Molecular Modeling applied to Biological Systems, National Laboratory of Scientific Computation, Petropolis, Brazil

2014 **Guest Lecture:** Molecular Dynamics Simulations of Large Systems, School of Molecular Modeling applied to Biological Systems, National Laboratory of Scientific Computation, Petropolis, Brazil

2014 **Workshop Teaching Assistant:** Hands-On Workshop on Computational Biophysics, Jacobs University, Bremen, Germany

2014 **Workshop Teaching Assistant**: Hands-On Workshop on Computational Biophysics, Ludwig-Maximilians-Universität München, Germany

2013 **Workshop Teaching Assistant:** Hands-On Workshop on Computational Biophysics, University of Illinois at Urbana-Champaign, Urbana

Referee/Reviewer

ACS Catalysis, ACS Central Science, BioData Mining, Biomolecules, Biotechnology and Bioengineering, Biotechnology for Biofuels, Computation, IEEE/ACM Transactions on Computational Biology and Bioinformatics, Current Proteomics, Energies, International Journal of Bioinformatics Research and Applications, International Journal of Molecular Sciences, Journal of Chemical Information and Modeling, Journal of Chemical Theory and Computation, Journal of Computational Physics, Journal of Molecular Modeling, Journal of Structural Biology, Materials, Molecular Biotechnology, Molecules, Nanomaterials, Pharmaceutics, PLOS One, RSC Advances, Scientific Reports, The Journal of Physical Chemistry

Professional Associations

- American Chemical Society
- Biophysical Society
- Brazilian Physical Society

Funding

Current

- NCSA/Blue Waters Allocation – 2019
  Title: Tackling the adhesion mechanism of antibiotic resistant pathogenic bacteria
  PI: Rafael C. Bernardi
  Amount: $322,400 equivalent in computer time
  Computer Time Amount: 520,000 node hours

Previous

- NSF/OAC ACI-1713784 – 2017 to 2019
  Title: The Computational Microscope
  PI: Emad Tajkhorshid
  Amount: $20,000.00
  Computer Time Amount: 17,650,000 node hours
  Role: co-PI

- DOE/ ASCR Leadership Computing Challenge (ALCC) – 2016 to 2017
  Title: Molecular Dynamics Studies of Biomass Degradation in Biofuel Production
  PI: Klaus Schulten
  Computer Time Amount: 50,000,000 processor hours
  Role: co-PI

- DOE/ ASCR Leadership Computing Challenge (ALCC) – 2015 to 2016
  Title: Molecular Dynamics Studies of Biomass Degradation in Biofuel Production
  PI: Klaus Schulten
  Computer Time Amount: 20,000,000 processor hours
  Role: co-PI

- DOE/ ASCR Leadership Computing Challenge (ALCC) – 2014 to 2015
  Title: Molecular Dynamics Studies of Biomass Degradation in Biofuel Production
  PI: Klaus Schulten
  Computer Time Amount: 69,000,000 processor hours
  Role: co-PI

Completed Research Support in Brazil (Role: PI)

- CNPq MCT/CNPq/Inmetro 059/2010 (563123/2010-9) – PROMETRO – 2011 to 2015
  Title: “Structural Analysis of Cellulose Chains and its Complex with Cellulases Employing Computational Modeling Methods”
  PI: Rafael C. Bernardi
  Amount: R$ 818,100.00 (~US$ 482,000.00 as of Dec 2010)

- ADT1/FAPERJ 2011 (E26/190.245/2011) – 2011 to 2012
  Title: “Computational Modeling Techniques Applied in the Development of Cellulose Chain Deconstruction for Second Generation Bioethanol Production”
  PI: Rafael C. Bernardi
  Amount: R$ 9,800.00 (~US$ 5,500.00)

- APQ5/FAPERJ 2011 (E-26/110.561/2011) – July 2011
  Special travel fund for participating in the 2011 World Congress of WATOC – Santiago de Compostela, Spain
  PI: Rafael C. Bernardi
  Amount: R$ 6,000.00 (~US$ 3,750.00)

List of References

1. **Prof. Emad Tajkhorshid**
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2. **Prof. Hermann Gaub**
   Faculty of Physics – Chair of Applied Physics
   Ludwig-Maximilians Universität München
   Amalienstraße 54
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   gaub@physik.uni-muenchen.de

3. **Prof. Edward Bayer**
   Department of Biological Chemistry
   Weizmann Institute of Science
   76100 Rehovot, Israel
   Phone: +972 (8) 934-2373
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Additionally:

4. **Prof. Michael Nash**
   Department of Chemistry – University of Basel &
   Department of Biosystems Science and Engineering – ETH Zurich
   Biopark Rosental 1096
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   4058 Basel, Switzerland
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5. **Prof. Zaida Luthey-Schulten**
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   University of Illinois at Urbana-Champaign
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   Department Molecular Theory and Spectroscopy
   Max Planck Institute for Chemical Energy Conversion
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7. **Prof. Gerd Rocha**
   Department of Chemistry
   Universidade Federal da Paraíba
   P.O. Box: 5093
   58051-970 João Pessoa, Brazil
   Phone: +55 (83) 3216-7590
   gbr@quimica.ufpb.br

26. SM Sedlak*, LC Schendel*, HE Gaub‡, RC Bernardi‡; *Streptavidin/biotin: tethering geometry defines unbinding mechanics*; **Science Advances**, accepted, **2019**

25. RC Bernardi‡*, E Durner*, C Schoeler, KH Malinowska, BG Carvalho, EA Bayer, Z Luthey-Schulten, HE Gaub, MA Nash‡; *Mechanisms of Nanonewton Mechanostability in a Protein Complex Revealed by Molecular Dynamics Simulations and Single-Molecule Force Spectroscopy*; **Journal of the American Chemical Society**, 141 (37), 14752-14763, **2019**

24. SM Sedlak*, LC Schendel*, MCR Melo, DA Pippig, Z Luthey-Schulten, HE Gaub, RC Bernardi‡; *Direction Matters – Monovalent Streptavidin/Biotin Complex under Load*; **Nano Letters**, 19 (6), 3415-3421, **2019** – *Cover Article*

23. TJK Haataja, RC Bernardi, S Lecointe, R Capoulade, J Merot, U Pentikäinen; *Non-syndromic Mitral Valve Dysplasia Mutation Changes the Force Resilience and Interaction of Human Filamin A*; **Structure**, 27(1), 102-112, **2019**

22. MCR Melo*, RC Bernardi*, T Rudack, M Scheurer, C Riplinger, JC Phillips, JDC Maia, GB Rocha, JV Ribeiro, JE Stone, F Neese, K Schulten, Z Luthey-Schulten; *NAMD goes quantum: A new integrative suite for hybrid simulations*; **Nature Methods,** 15 (5), 351-354, **2018**

21. LF Milles, K Schulten, HE Gaub, RC Bernardi‡; *Molecular mechanism of extreme mechanostability in a pathogen surface anchor*; **Science**, 359 (6383), 1527-1533, **2018**

20. M Scheurer, P Rodenkirch, M Siggel, RC Bernardi, K Schulten, E Tajkhorshid, T Rudack; *PyContact: Rapid, Customizable and Visual Analysis of Non-Covalent Interactions in MD Simulations*; **Biophysical Journal**, 114(3), 577-583, **2018** – *Cover Article*

19. T Verdorfer, RC Bernardi, A Meinhold, W Ott, Z Luthey-Schulten, MA Nash, HE Gaub; *Combining in Vitro and in Silico Single Molecule Force Spectroscopy to Characterize and Tune Cellulosomal Scaffoldin Mechanics*; **Journal of The American Chemical Society**, 139 (49), 17841-17852, **2017** – *Cover Article*

18. J Seppälä, RC Bernardi, TJK Haataja, M Hellman, OT Pentikäinen, K Schulten, P Permi, J Ylänne, U Pentikäinen; *Skeletal Dysplasia Mutations Effect on Human Filamins' Structure and Mechanosensing*; **Scientific Reports**, 7 (1), 4218, **2017**

17. JV Ribeiro*, RC Bernardi*, T Rudack*, JE Stone ,JC Phillips,PL Freddolino, K Schulten; *QwikMD Integrative Molecular Dynamics Toolkit for Novices and Experts*; **Scientific Reports**, 6, 26536, **2016**

16. BC Goh*, JA Hadden*, RC Bernardi, A Singharoy, R McGreevy, T Rudack, CK Cassidy, K Schulten; *Computational Methodologies for Real-Space Structural Refinement of Large Macromolecular Complexes*; **Annual Review of Biophysics**, 45, 253-278, **2016**

15. I Cann, RC Bernardi, RI Mackie; *Cellulose degradation in the human gut: Ruminococcus champanellensis expands the cellulosome paradigm*; **Environmental Microbiology**, 18 (2), 307-310, **2016**

14. C Schoeler*, RC Bernardi*, KH Malinowska, E Durner, W Ott; EA Bayer; K Schulten; MA Nash; HE Gaub; *Mapping mechanical force propagation through biomolecular complexes*; **Nano Letters**, 15 (11), 7370-7376, **2015** – *Cover Article*

13. RC Bernardi, MCR Melo, K Schulten; *Enhanced Sampling Techniques in Molecular Dynamics Simulations of Biological Systems*; **Biochimica et Biophysica Acta (BBA) – General Subjects**, 1850 (5), 872-877, **2015**

12. JR Perilla, BC Goh, CK Cassidy, B Liu, RC Bernardi, T Rudack, H Yu, Z Wu, K Schulten; *Molecular dynamics simulations of large macromolecular complexes*; **Current Opinion in Structural Biology**, 31, 64-74, **2015**

11. C Schoeler*, KH Malinowska*, RC Bernardi, LF Milles, MA Jobst, E Durner, W Ott, DB Fried, EA Bayer, K Schulten, HE Gaub, MA Nash; *Ultrastable cellulosome-adhesion complex tightens under load*; **Nature Communications**, 5, 5635, **2014**

10. RC Bernardi, I Cann, K Schulten; *Molecular dynamics study of enhanced Man5B enzymatic activity*; **Biotechnology for Biofuels**, 7 (1), 83, **2014**

9. YS Mendes*, NS Alves*, TLF Souza, IP Sousa, ML Bianconi, RC Bernardi, PG Pascutti, JL Silva, AMO Gomes, AC Oliveira*; The Structural Dynamics of the Flavivirus Fusion Peptide-Membrane Interaction*; **PloS one**, 7 (10), e47596, **2012**

8. MCR Melo, RC Bernardi‡, TVA Fernandes, PG Pascutti; *GSAFold: A new application of GSA to protein structure prediction*; **Proteins: Structure, Function, and Bioinformatics**, 80 (9), 2305-2310, **2012**

7. RC Bernardi‡, PG Pascutti; *Hybrid QM/MM Molecular Dynamics Study of Benzocaine in a Membrane Environment: How Does a Quantum Mechanical Treatment of Both Anesthetic and Lipids Affect Their Interaction*; **Journal of Chemical Theory and Computation**, 8 (7), 2797-2203, **2012**

6. LVB Hoelz, AAST Ribeiro, RC Bernardi, BAC Horta, MG Albuquerque, JFM Silva, PG Pascutti, RB Alencastro; *The role of helices 5 and 6 on the human β1-adrenoceptor activation mechanism*; **Molecular Simulation**, 38 (3), 236-240, **2012**

5. LVB Hoelz, RC Bernardi, BAC Horta, JQ Araújo, MG Albuquerque, JFM Silva, PG Pascutti, RB Alencastro; *Dynamical behaviour of the human β1-adrenoceptor under agonist binding*; **Molecular Simulation**, 37 (11), 907-913, **2011**

4. RC Bernardi, DEB Gomes, R Gobato, CA Taft, AT Ota, PG Pascutti; *Molecular dynamics study of biomembrane/local anesthetics interactions*; **Molecular Physics**, 107 (14), 1437-1443, **2009**

3. RC Bernardi, DEB Gomes, AS Ito, AT Ota, PG Pascutti, C Taft; *Density functional and molecular dynamics simulations of local anesthetics in 0.9% NaCl solution*; **Molecular Simulation**, 33 (14), 1135-1141, **2007**

2. RC Bernardi, DEB Gomes, PG Pascutti, AS Ito, CA Taft, AT Ota; *Water solvent and local anesthetics: A computational study*; **International Journal of Quantum Chemistry**, 107 (7), 1642-1649, **2007**

1. RC Bernardi*, DEB Gomes, PG Pascutti, AS Ito, AT Ota*; Theoretical studies on water-tetracaine interaction; **International Journal of Quantum Chemistry**, 106 (5), 1277-1282, **2006**

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