

Dr. Rafael C. Bernardi

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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**
- 2010-2013 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 Affairs 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

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 of Non-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 compared 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 compared 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 compared 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 compared 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 compared 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 compared 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 – Aug **NAMD Developer Workshop**, Urbana, IL, USA
- 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 – Aug **NAMD Developer Workshop**, Urbana, IL, USA
- 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 – May **NAMD Developer Workshop**, Chicago, IL, 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, Pharmaceuticals, 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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Additionally:

4. **Prof. Michael Nash**
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27. SM Sedlak*, LC Schendel*, HE Gaub†, RC Bernardi‡; *Streptavidin/biotin: tethering geometry defines unbinding mechanics*; **Science Advances**, accepted, **2020**
26. I Cann, GV Pereira, AM Abdel-Hamid, H Kim, D Wefers, BB Kayang, T Kanai, T Sato, RC Bernardi, H Atomi, RI Mackie; *Thermophilic degradation of hemicellulose, a critical feedstock in the production of bioenergy and other value-added products*; **Applied Environmental Microbiology**, accepted, **2020**
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 Yläne, 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; *Ultraprecise cellulose-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 β 1-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 β 1-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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† Corresponding Author