

Clemson University

Emil Alexov

PERSONAL DATA

Professor
Department of Physics
Clemson University
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EDUCATION

Ph.D., Sofia University, 1990, Radio-physics and Electronics
M.S., Sofia University, 1984, Plasma Physics

PROFESSIONAL EXPERIENCE

American Institute for Medical and Biological Engineering (AIMBE) Fellow (2025 – now)
Clemson University (2025 – now), College of Science Dean Distinguished Professor
Clemson University and PrismaHealth (2021-2024), Roy Wallace Distinguished Professor, USA
Clemson University (2012 – now), Professor, Department of Physics
Clemson University (2018 – new), Professor, School of Nursing: Healthcare Genetics
Clemson University (2015 – now), Faculty Scholar, School of Health Research
Clemson University (2015 – now), Professor, Department of Material Sciences
University of Alabama (2018 – 2027); Graduate Faculty at The University of Alabama
Clemson University (2005 – 2012), Associate Professor, Department of Physics
Howard Hughes Medical Institute and Columbia University, New York (2000-2005), Senior Scientist
Bronx Community College, New York (1997-2005), Adjunct Assistant Professor
City College of New York (1995-2000), Research Associate
The Institute of Physical and Chemical Research (RIKEN), Japan (1994-1995), Visiting Scientist
Bulgarian Academy of Sciences (1992-1994), Staff Scientist
Medical Academy, Bulgaria (1991-1992), Assistant Professor
Sofia University, Bulgaria (1990-1991), Assistant Professor

HONORS AND AWARDS

2025 University Research, Scholarship and Artistic Achievement Award, Clemson, USA
2018 Alumni Award for Outstanding Achievement in Research, Clemson, USA
2015 Faculty Achievement in Science, Clemson University, USA
2014 Faculty Scholar at the School of Health Research, Clemson, USA
2013 Outstanding Graduate Student Mentor, Clemson University, USA
2004 Science and Technology Agency Award (STA Fellowship), Japan

MEMBERSHIPS

Member, American Physical Society (1990)
Member, American Chemical Society (2007)
Member, Biophysical Society (1995)
Member, Protein Society (1995)

PROFESSIONAL ACTIVITIES

National Institutes of Health (NIH), NIH ZRG1 BST-Q section (2008-2009); NIH ZRG1 IMST-A (2009), NIH BDMA (2010 – 2012, 2015-2017), NIH MSFD (2010), NIH ZCA1 SRB-X (2018), NIH BCMB (2018), NIH BST IRG (2018), NIH ZRG1 BST (2018), NIH ZCA1 SRB-X (2019), NIH ZRG1 BCMB-G (2019). ZCA1 RTRB-R (M3) NCI Special Emphasis Panel - Information Technology in Cancer Research (2021), Cancer research section (2022), ZCA1 TCRB-9 (M1) (2024), ZDC1 SRB-K (13) (2024), 2024/10 ZRG1 MGG-K (02) M: Molecular Genetics and Genomics (2024), 05 ZDC1 SRB-K (13) L (2024).

National Science Foundation (NSF), Panel Member: CDI (2010), MCB (2010-2017), DMS (2017), Chemistry Of Life Processes Program (2023).

American Chemical Society: ACS PRF Proposal Review No. 62121-ND 6 (2021).

Cottrell College Science Award, mail reviewer, 2010.

Canada: New Frontiers in Research Fund (NFRF) (2022), OICR (2023), OICR Investigator Award (2024)

Europe: Irish Research Foundation (2007-2008), and the National Center for Scientific Research (CNRS) ANR-PCV (France) (2007), CNRS (2017), UKRI BBSRC – United Kingdom (2021)

MEETING ORGANIZER

Co-organizer: Symposium “Electrostatics and polarization in inhomogeneous media: Physico-chemical effects at the interface of macromolecule-water phases”, Annual Meeting of American Chemical Society, Denver, 2024.

Co-organizer: Symposium, “Barry Honing 80th birthday symposium”, San Diego, 2022.

Co-organizer: Symposium, “Modeling effect of mutations on macromolecular stability and binding”, Annual Meeting of American Chemical Society, San Diego, 2021.

Co-organizer: Symposium, “Role of Water Phase in Molecular Biology: Importance of Water in Folding, Binding & Transport Phenomena”, Annual Meeting of American Chemical Society, San Diego, 2019

Co-organizer: Symposium, “Molecular recognition: Revealing the effects associated with receptor-ligand binding”, Annual Meeting of American Chemical Society, Washington, 2017

Co-organizer: Symposium, “Revealing the Role of Water in Calculations of Solvation Energy”, Annual Meeting of American Chemical Society, Philadelphia, 2016

Co-organizer: Mathematical Biomedical Institute “Emphasis Year on Mathematical Molecular Biosciences”, 2015, Columbus, OH. This includes: Workshop 1: “Geometric and Topological Modeling of Biomolecules” September 28, 2015 - October 02, 2015; Workshop 2: “Multiple Faces of Biomolecular Electrostatics” October 12, 2015 - October 16, 2015; Workshop 3: “Modeling and Computation of Transmembrane Transport”, November 16, 2015 - November 20, 2015; and Workshop 4: “Mathematical Challenges in Drug and Protein Design”, December 07, 2015 - December 11, 2015.

Co-organizer: Gordon Research Conference “Human Single Nucleotide Polymorphisms & Disease”, 2014, Aug 3-8, Stonehill College, MA.

Co-organizer: Symposium, “Interplay Between Forces in Biochemistry”, Annual Meeting of American Chemical Society, Boston, 2015.

Co-organizer: Symposium, "Molecular Biophysics", Annual Meeting of American Chemical Society, San Francisco, 2014.

Co-organizer: Symposium, "Electrostatic and Polarization Effects in Physical Chemistry: *In silico and in vitro*", Annual Meeting of American Chemical Society, Indianapolis, 2013.

Co-organizer: Symposium, "Modeling Solvation in Molecular Biology", Annual Meeting of American Chemical Society, Philadelphia, 2012.

Organizer: "Modeling Electrostatics in Molecular Biology", Clemson, 2011

Co-organizer: "pKa cooperative initiative". Telluride, 2009 and 2011.

Organizer: "eCheminfo 2008", Platform Organizer and Chair, Bryn Mawr, 2009.

Organizer: "3rd Bioinformatics Symposium", Clemson, 2007.

INVITED TALKS (the most recent)

Protein Electorstatics, DelPhiForce molecular dynamics simulations. Telluride (2024).

CaGI-6 (Critical Assessment of Genome Interpretation), invited talk on SAAFEC-SEQ. Winner in MARK challenge. (2023)

SIAM Annual Meeting, July 11 - 15, 2022, invited talk "Multi-scale modeling of microtubule binding domain (MTBD) association with microtubule", Pittsburgh, PA, (2023)

Invited talk, Queens University, Canada "Do thermodynamics and pathogenicity like each other? Case study of X-linked monogenic diseases", Sept. 20, 2022.

Mathematical Molecular Biosciences (MMB), "Energy and pathogenicity: Case study of X-linked monogenic diseases", Oct. 5, 2022.

"DelPhi: New developments and review of functionalities", Annual meeting of ACS, San Diego, 2022.

"Reproducing ensemble averaged quantities": NSF-CBMS Conference: Mathematical Molecular Biosciences and Biophysics, May 13- 17, 2019. University of Alabama.

"Modeling the role of electrostatics in macromolecular recognition": Oct. 3-5, 2019. seminar at University of Texas at El Paso.

"Super-Gaussian smooth dielectric for macromolecular modeling": Tsinghua Sanya International Mathematics Forum (China) Dec 8-12, 2019.

"Disease-causing mutation in MePC2 protein affecting protein-DNA binding", INSERM, France, April 2018.

"Physics-based approaches in molecular biology and their applications to reveal the mechanism of human diseases", Auburn University, February 11, 2017.

"Multi-scale Modeling of Kinesin and Dynein Binding to Microtubules", Yau Mathematical Sciences Center, China, December 22, 2016.

"Revealing molecular mechanism of mono genetic disorders and targeting disease-causing effects with small molecule binding", Vanderbilt University, TN, April 22, 2016.

"Targeting disease-causing effects with small molecules binding", MBI Emphasis Semester on Mathematical Molecular Biosciences, Dec. 6-11, 2015, MBI, Ohio, USA.

<https://mbi.osu.edu/video/player/?id=3772&title=Targeting+disease-causing+effects+with+small+molecules+binding>

“Modeling Electrostatics in Biological Membranes and Membrane Proteins: Applications to Human Diseases”, MBI Emphasis Semester on Mathematical Molecular Biosciences, Nov. 18-24, 2015, MBI, Ohio, USA.

“Modeling Macromolecular Electrostatics with DelPhi Poisson-Boltzmann solver: Development and applications”, invited talk at Tianjin University, October 21, 2015, Beijing, China.

“Snyder-Robinson syndrome: molecular mechanism and rescuing the effect with small molecules”, Drug Discovery and Innovations, October 2-22, Beijing, China 2015.

“pKa calculations without defining molecular surface”, Protein electrostatics, July 8-12, 2015, Telluride, USA.

“Rett Syndrome Causing Mutations in MeCP2”, invited talk at University of Paris 7, April 28, 2015, Paris, France,

“Revealing molecular mechanism of Snyder-Robinson Syndrome and rescuing it with small molecule binding”, May 19, 2015, ORNL, USA.

“Listen to your genes”, May 8, 2015, TED talk. <https://www.youtube.com/watch?v=BY7ZziM28UQ>

“Electrostatics in Molecular Biology”, 2014 International Symposium on Laser and Computational Biophysics, June 15-17, Shanghai, China, 2014.

“Modeling Macromolecular Electrostatics with DelPhi Poisson-Boltzmann solver: Improvements and applications”, Oregon State University, October, 2014.

“Structure-based modeling of the effects of missense mutations associated with human disorders”, Genomics-2014, Raleigh, NC, September, 2014.

“Modeling Electrostatics in Molecular Biology via DelPhi Poisson-Boltzmann solver: Improvements and applications, NIH, April 7, 2014.

“Targeting diseases with small molecule rescuers”, NIH, May 8, 2014

REVIEWER

Reviewer for Journal of Molecular Biology, Journal of Physical Chemistry, Proteins, Bioinformatics, Protein Science, Journal of Molecular Graphics, Computational Biology, Biophysical Journal, European Biophysical Journal, European Biochemistry Journal, Biochemistry, Journal of Computational Chemistry, PNAS, Protein Engineering, etc.

EDITOR

Editor-in-Chief of Journal of Computational Biophysics and Chemistry

Guest Editor for International Journal of Molecular Sciences

Guest Editor: Genes

Guest Editor for Journal of Molecular Biology

Guest Editor for Communications in Computational Physics

Guest Editor for Current Biotechnology Journal

Associate Editor of Physical Review & Research International

Associate Editor of Computational and Mathematical Methods in Medicine

Associate Editor of Frontiers Molecular Biosciences

EDITORIAL BOARD MEMBER

Chemical Physics Letters

SOFTWARE and WEBSERVERS

The computer codes are downloadable and webserver accessible free of charge from our webpage (compbio.clemson.edu → Software & Webserver). Below we briefly outline the features associated with each development.

- **DelPhi software:** DelPhi C++ is an Object-Oriented (OO) program that computes the 3D distribution of electrostatic potential in proteins, RNAs, DNAs and nano objects. Once the potential is calculated, the corresponding electrostatic energy components are also delivered. The program is developed for Linux, Mac and Windows. <http://compbio.clemson.edu/delphi>
- **DelPhi webserver:** To further facilitate the DelPhi usage, we developed a DelPhi webserver, with which inexperienced users may submit their jobs without having to familiarize themselves with the DelPhi stand-alone program http://compbio.clemson.edu/sapp/delphi_webserver/. Through self-navigating system with a help menu, the server provides all necessary parameter files for a DelPhi run. Using the embedded ProNOI, users may model both the biological macromolecules and various nano-particles of their choice.
- **DelPhiPKA:** Webserver to predict pKa's of proteins, RNAs and DNAs. The pKa method was tested against two large databases of experimentally determined pKa's (PPD database: 34 proteins with 302 titratable residues and pKa-cooperative database: SNase mutants of 109 pKa's). The datasets include variety of cases from strongly coupled titration sites to almost isolated but deeply buried sites. The overall benchmarking over three different force field parameters (Amber, Charmm and OPLS) resulted in RMSD=0.78pK and RMSD=1.6pK for PPD and pKa-cooperative databases, respectively. The preliminary results are among the top in the field. The method is implemented into a webserver, which is easy to navigate and provides various outputs, including predicted pKa's and a structure with proton position assigned at user specified pH. The method and the webserver allows for predicting pKa's of proteins, RNAs and DNAs. Link: http://compbio.clemson.edu/pka_webserver/
- **BION webserver:** We developed an algorithm that predicts the position of non-specifically bound ions on the surface of proteins. The algorithm utilizes Delphi calculated potential map in conjunction with in-house developed clustering algorithm to predict non-specific ion binding sites. The approach was benchmarked against experimentally determined non-specifically bound ions and it was shown that the predictions are of good accuracy. The algorithm is now implemented in a webserver http://compbio.clemson.edu/bion_server/.
- **ProBLM webserver:** The server allows the users to upload their structural file in PDB format, to select either explicit or implicit membrane and then the server automatically positions the protein into a membrane. The webserver is complemented with Jmol visualization and allows users to manipulate the position and the orientation of the protein within membrane via sliders http://compbio.clemson.edu/sapp/problm_webserver/.
- **ProNOI software:** many important targets for modeling as neurons, endoplasmic reticulum, Golgi apparatus and other nano-scale objects are irregularly shaped. To overcome this problem, we developed an approach to model geometrical objects as objects made of pseudo-atoms. The first version of the corresponding algorithm, the ProNOI is available for free download

<http://compbio.clemson.edu/pronoi>. Essentially, the ProNOI allows the users to generate a PDB-format file of unlimited number of objects and proteins together. The objects that ProNOI generates are parallelepiped, sphere, cone and cylinder. The next generation of ProNOI, ProNOI-2, is much more complex in that the users may create a 3D presentation from a 2D photograph. This development was inspired by our plans to model cellular organelles, neurons and other entities seen in Cryo-electron Microscopy (cryo-EM) or another experimental technique. Two scenarios are considered: (a) the user is provided with series of photos (in x-y plane) taken at different depths (different z-coordinate values); and (b) the user is provided with only one photo taken at a particular z-coordinate value. In the first scenario, the user utilizes ProNOI-2 to trace the object(s) of each photo, and manually specifies the corresponding z-coordinate value and combines the individual files generated by ProNOI-2 into a single PDB-format file. In the second scenario, the user must decide the symmetry of the objects along z-axis and model the object according the presumed symmetry. The ProNOI-2 gives the users the option of selecting the charge and dielectric constant for each generated object.

- **SAAMBE webserver:** Single Amino acid Mutation related change of Binding Energy (SAAMBE) is a webserver, which addresses the demand for computational tools of predicting the effect of single amino acid substitution on the binding free energy of protein complexes. It is based on the fast (< 1 minute) modified MM-PBSA protocol that is successfully tested and optimized for more than thousand experimental data points from SKEMPI database. Link: http://compbio.clemson.edu/saambe_webserver/

- **SAAFEC Webserver:** Single Amino Acid Folding free Energy Changes (SAAFEC) is an approach for calculating folding free energy changes caused by missense mutations. The method is based on weighted MM-PBSA method with weight coefficients optimized against experimental data from the ProTherm database. Furthermore, the prediction formula is extended to include various biophysical terms to enhance the performance. Link: <http://compbio.clemson.edu/SAAFEC/>

- **Multi-Scale Simulation Package (MSSM):** The multi-scale approach is capable of modeling the binding process between large and small biological objects. Examples include but are not limited to motor domain binding to microtubules, protein binding to viruses, protein binding to a membrane and many others. The MSSP is comprised of three main modules: (1) sampling module, (2) energy calculation module and (3) Monte Carlo and path generation module. The first module, module 1, generates multiple conformations of the small object around the large one. The module utilizes cuboidal, spherical, and cylindrical sampling distributions. The second module, module 2, calculates electrostatic and van der Waals energies. Because calculating the electrostatic potential of biological molecules and assemblages is the most complex and intensive computational task, it represents the bottleneck in performing computations on large systems. The MSSP specifically targets efficiency improvements in the electrostatic energy calculations. We developed a novel algorithm that first calculates electrostatic energy at a coarse-grained resolution in the entire system. Then it transfers the information from the entire environment to a focused local region of interest and calculates the electrostatic energy at a significantly finer resolution. The third module, module 3, applies Monte Carlo procedure to evaluate the probabilities of each generated conformation and then restore the plausible pathway of small object binding onto the large one.

- **SAMPDI Web Server:** It provides fast and accurate predictions for the effects of single amino acid substitution on the binding free energy of protein-DNA complex. This method utilizes modified molecular mechanics Poisson-Boltzmann Surface Area (MM/PBSA) approach along with an additional set of knowledge-based terms delivered from investigation of the physico-chemical properties of protein-DNA complexes. Important feature is applying DelPhi Gaussian-based smooth dielectric function to calculate the change of solvation energy. <http://compbio.clemson.edu/SAMPDI/>

- **DelPhiForce Web Server:** Delphi Force is a DelPhi-based script, allowing to calculate the electrostatic force between two objects, such as proteins, DNAs, lipids, small molecules, etc. <http://compbio.clemson.edu/delphi-force/>

- **Intellectual Properties (IP):**

- a. IP. Tech ID: 2013-018; IR: 1626401-12-0015; Algorithms and Computer Code for Parallel Computing of Electrostatics in Systems Made of Biological Macromolecules and Objects; Grant support: GM093937, National Institutes of Health; PI: E Alexov ; Disclosure date: 2012-08-13.
- b. IP. Tech ID: 2013-0211; IR: 626401-12-0017; Gaussian Dielectric Function in DelPhi; Grant Sponsor: GM093937, National Institutes of Health; PI: E. Alexov; Disclosure date: 2012-08-14.
- c. IP; Tech ID: 2013-0201; IR: 626401-12-0016; ProNOI software; Grant Sponsor: GM093937, National Institutes of Health; PI: E. Alexov; Disclosure date: 2012-08-14.
- d. IP; Tech ID: 2016-0036; IR: 626401-15-0045; Multi-scale simulation package (MSSM); Grant Sponsor: GM093937, National Institutes of Health; PI: E. Alexov; Disclosure date: 2016-03-26.
- e. IP; Tech ID: 2016-0037; IR: 626401-15-0048; DelPhiPKA; Grant Sponsor: GM093937, National Institutes of Health; PI: E. Alexov; Disclosure date: 2016-03-26.

SPONSORED RESEARCH

Ongoing Research support

R35GM151964	Alexov (PI)	02/01/2024 – 01/31/2029
NIH/NIGMS		
DePhi and associated resources: maintenance, development and applications		

This grant support further development and maintenance of DelPhi, a popular software package for modeling electrostatic potential and energies in systems made of biological macromolecules, the associated resources for predicting folding and binding free energies caused by mutations and to apply these resources to investigate molecular mechanism of human diseases.

NSF	(Zhao)	10/01/2025 – 09/31/2028
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NSF DMS/Mathematical Biology

Collaborative Research: On calculating polar solvation and binding energies for non-rigid proteins in the Poisson-Boltzmann theory: modeling, analysis and applications.

Role: Co-PI

NSF	(Podila)	10/01/2025 – 09/31/2029
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IGE: Track 2: AI-Driven Virtual Teaching Assistant (ViTA) in Medical Biophysics Graduate Education

Role: Co-PI

Completed

R01GM093937	Alexov (PI)	03/01/2022 – 02/28/2024
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NIH/NIGMS

Development and maintenance of DelPhi and associated resources

This grant supports further development and maintenance of DelPhi, a popular software package for modeling electrostatic potential and energies in systems made of biological macromolecules and geometrical shapes, and associated resources.

Role: PI

1R01GM125639

Yu (PI)

01/23/2018 – 12/31/2022

NIH/NIGMS

Quantifying molecular consequences of human missense variants with large-scale interactome perturbation studies

This grant supports development of methods and computer code to predict effects of mutations on protein-protein binding free energy.

Role: Co-PI

NSF

(Zhao)

8/15/2018 – 7/31/2022

NSF DMS/Mathematical Biology

Collaborative Research: A Regularized Poisson Boltzmann Model for Fast Computation of the Ensemble Average Polar Solvation Energy

The major goal of this project is to develop super Gaussian approach to compute solvation energy of biomolecules

Role: Co-PI

NIH

Yao (PI)

09/15/18 - 07/31/2023

SC COBRE for Musculoskeletal Health Translational Research

Role: Mentor

Collaborative Linkage Grant

Alexov(PI)

06/01/1999 – 05/31/2001

NATO

Proton transport in Reaction Center protein

This is a collaborative grant with France, to investigate by combined means of *in silico* and *in vitro* approaches the effects of single point mutations of the wild type properties of Reaction Center protein.

Role: PI

Collaborative Linkage Grant

Alexov(PI)

06/01/2002 – 05/31/2004

NATO

Plastocyanin polymorphism

This is a collaborative investigation with Bulgaria and France, both computationally and experimentally to reveal the biological significance of plastocyanin dimorphism.

Role: PI

Collaborative Linkage Grant

Alexov(PI)

06/01/2005 – 05/31/2006

NATO

Bioinformatics

This is a collaborative grant to help our Bulgarian partner to enter the area of Bioinformatics. It provided training and donation of equipment for Bulgarian laboratory.

Role: PI

Collaborative Linkage Grant

Alexov(PI)

06/01/2010 – 05/31/2011

NATO

Developing a novel method for rapid detection of small organic molecules

This is a collaborative grant with Sweden and Russia to test the possibility of using lysozyme internal motion to detect small organic molecules by the means of monitoring lysozyme GHz absorption profile.

Role: PI

R03 LM009748

Alexov(PI)

07/01/2009 – 06/30/2012

NIH/NLM

The effect of single nucleoside polymorphism on protein structure and interactions

This grant supports *in silico* investigations of the molecular effects associated with Snyder-Robinson Syndrome and how missense mutations affect the wild type characteristics of Spermine Sythase protein.

Role: PI

R03 LM009748-S1

Alexov(PI)

07/01/2010 – 06/30/2012

NIH/NLM

The effect of single nucleoside polymorphism on protein structure and interactions

This is a supplement of the above grant to allow for experimental investigations of the effects predicted *in silico* on the wild type characteristics of Spermine Sythase protein.

Role: PI

Institutional grant (Clemson University) Alexov (PI)

01/01/2014 – 01/31/2016

The Biology of Human Diseases

The grant provided funds for three postdoctoral researchers and supplies to carry research on developing drugs to treat mental disorders associated with SNPs in MeCP2 and KDM5C proteins.

Role (PI)

R01GM093937

Alexov (PI)

08/10/2011 – 07/31/2016

NIH/NIGMS

DelPhi: software for modeling electrostatic potential in biomolecules and objects

This grant support maintenance and further development of DelPhi, a popular software package for modeling electrostatic potential and energies in systems made of biological macromolecules and geometrical shapes.

Role: PI

R01GM093937

Alexov (PI)

05/15/2016 – 02/29/2021

NIH/NIGMS

New Generation DelPhi: Large objects and beyond electrostatics

This grant support further development of DelPhi, a popular software package for modeling electrostatic potential and energies in systems made of biological macromolecules and geometrical shapes, to include modeling on non-electrostatic quantities and ability to compute large objects of size > 1000A.

Role: PI

NSF

Alper (PI)

05/15/2019 -

05/14/2020

REU

Nature's machinery through the prism of physics, biology, chemistry and engineering

Role: Co-I

NIH: R15

Alper (PI)

07/01/2018 -06/30/2020

Targeting flagellar motility in the treatment of kinetoplastid diseases

Role: Co-I

VISITING FACULTY/POSTDOC/GRADUATE STUDENT ADVISING

Visiting Faculty

In Clemson: Prof. Thereza Soares (Brazil)
Dr. Petya Christova (Bulgarian Academy of Sciences)
Dr. Alexandra Shosheva (Bulgarian Academy of Sciences)
Dr. Victor Morozov (Russian Academy of Sciences)
Before Clemson: Dr. Pierre Sebban (CRNS, France)
Dr. Mitko Dimitrov (Bulgarian Academy of Sciences)
Dr. Antony Donchev (Bulgarian Academy of Sciences)

Postdoctoral Associates Advised

Dr. Petras Kundrotas, Dr. Daquan Gao, Dr. Maxim Zhenirovskyy, Dr. Chuan Li, Dr. Lin Li, Dr. Tugba Kucukkal, Dr. Zhe Jia, Dr. Sankar Basu, Dr. Swagata Pahari, Dr. Gen Li, Dr. Bohua Wu, Dr. Preeti Pandey, Dr. G. Munees

Current Postdoctoral Associates Advising

Dr. Shailesh Pandey

Graduate students advised

Mahesh Koirala, PhD, 2022, "Modeling electrostatics in molecular biology and its relevance with molecular origin of diseases"

Mihiri Hewa Bosthanthirige, PhD, "Revealing the role of electrostatics in molecular recognition, ion binding and pH-dependent phenomena"

Shannon Bonomi, MS, 2021, "Prediction of pathogenic mutations in spermine/spermidine synthases"

Satishkumar Ranganathan Ganakammal, PhD, 2020, "Genetics in Healthcare".

Nayere Tajielyato, PhD, 2020, "Modeling protein-protein binding and folding"

Bohua Wu, PhD 2020, "Association between MSH2 missense mutations and breast cancer"

Arghya Chakravorty, PhD, 2019, "Modeling Electrostatics and Geometrical Quantities In Molecular Biophysics Using a Gaussian-Based Model of Atoms". The student was awarded the "**Outstanding Graduate Researcher Award**" of the Department of Physics and Astronomy.

Yunhui Peng, Clemson University, PhD, 2018, "Developing method and algorithms for modeling effects of mutations associated with diseases". The student was awarded the "**Outstanding**

Graduate Researcher Award” at all levels: Clemson University, College of Sciences and Department of Physics and Astronomy.

Lin Wang, Clemson University, PhD, 2015, “Developing methods for pKa predictions for proteins, DNAs and RNAs”.

Marharyta Petukh, Clemson University, PhD, 2015, “Developing methods for ion prediction and applications to human diseases”. The student was awarded the “**Outstanding Graduate Researcher Award**” at all levels: Clemson University, College of Sciences and Department of Physics and Astronomy.

Nicholas Smith, Clemson University, MS, 2015, “Protein Nano-Object Integrator (ProNOI)”.

Shannon Stefl, Clemson University, MS, 2015, “Revealing molecular mechanism of Snyder-Robinson Syndrome”.

Zhe Zhang, Clemson University, Dual PhD: PhD in Physics from Clemson University and PhD in Life Sciences from University of Paris, France, 2013. “Understanding molecular effects of mental disorders”. The student was awarded the “**Outstanding Graduate Researcher Award**” at all levels: Clemson University, College of Sciences and Department of Physics and Astronomy.

Rooplekha Mitra, Clemson University, 2010, MS. “Modeling proton uptake/release in protein-protein interactions”.

Paulina Georgieva, Bulg. Academy of Sciences, 2009, PhD. “Mono-phosphate kinases – experimental and computational studies”.

Current PhD Student Advising

Prawin Rimal, Pitambar Poudel, Nirav Modha, Shamrat Paul

TEACHING

Courses Taught in Clemson University (Beginning Spring 2006)

PHYS 418, Modern Physics, S06

PHYS 311: Mathematical Methods for Theoretical Physics, F06, F07, F08

PHYS 417: Introduction to Biophysics, F06

PHYS 312: Mathematical Methods for Theoretical Physics, S07, S08, S09

PHYS 811: Mathematical Methods for Physicists, F10.

PHYS 812: Mathematical Methods for Physicists, S11.

PHYS 875: Computational Biophysics, F11.

PHYS 417: Intro to Biophysics, F12

PHYS 200: General Physics, S13

PHYS 875: Human DNA variants and diseases, F13

PHYS 819: Computational Biophysics, F14

PHYS 875: Human DNA variants and diseases, S15

PHYS 315: Introduction to computational physics, F15

PHYS 819: Human DNA variants and diseases, S16

PHYS 315: Introduction to computational physics, F16

PHYS 819: Computational Biophysics, S17

PHYS 315: Introduction to computational physics, F17

PHYS819: Computational Biophysics, S2018
 PHYS 315: Introduction to computational physics, F18
 PHYS 819, Computational Biophysics, S2019
 PHYS 315: Introduction to computational physics, F19
 PHYS122: Physics with calculus, S20
 PHYS 819: Computational Biophysics, F20
 PHYS 120: Physics with Calculus, S21
 PHYS 819: Computational Biophysics, F21
 PHYS 122: Physics with calculus, S22
 PHYS 1220: Physics with calculus, F22
 MBIO 8100: Medical Biophysics core 1, F22
 MBIO 8110: Medical Biophysics core 2, F22
 MBIO 8210: Medical Biophysics core 3; S23
 MBIO B220: Medical Biophysics core 4, S23
 MBIO 8100: Medical Biophysics core 1, F23
 MBIO 8110: Medical Biophysics core 2, F23
 MBIO 8210: Medical Biophysics core 3; S24
 MBIO B220: Medical Biophysics core 4, S24
 PHYS 8190: Computational Biophysics, S24
 MBIO 8100, Medical Biophysics, F24
 MBIO 8110, Medical Biophysics, F24
 MBIO 8210, Medical Biophysics, S25
 MBIO 8220, Medical Biophysics, S25
 MBIO 8100, Medical Biophysics F25
 MBIO 8110, Medical Biophysics, F25

Courses Taught in Bronx Community College, New York

Introductory Astronomy, each semester from 1997 until 2005. Lecture and labs.

Courses Taught in City College of New York

Classical Mechanics, Seminars, 1998-1999.

Courses Taught in Medical Academy, Bulgaria

Medical Physics, F1991, S1992.

Courses Taught in Sofia University, Bulgaria

Quantum Mechanics, F1990, S1991.

Courses Taught in Technical Institute, Bulgaria.

Engineering Physics, F1990.

UNIVERSITY AND PUBLIC SERVICE

Committees

Chair: Medical Biophysics Admission Committee (2022-)
 Chair: Medical Biophysics Curriculum Committee (2022-)
 Chair: Millers' Endowed Chair Search Committee (2021-)
 Chair: College Election Committee (2019-)
 Member: College Discovery Committee (2018-)

Chair: Strategic PhD program (2019-)
Chair: Personnel Committee (2018-)
Member: Strategic Planning Committee (2013-)
Member: Department Advisory Committee (2011-)
Member, Committee to Review Department By-Laws (2005-)
Chair, Biophysics Faculty Search (2006), Member (2012, 2014)
Member, Graduate Student Evaluation Committee, (2006-2008, 2015-)
Member, Faculty Advisory Committee (2008-)

New graduate program: Established new MS/PhD program in Medical Biophysics which is currently offered at Fall 2022.

Organizer and narrator of “Biophysics and Bioinformatics” seminars for graduate students, here in Clemson (2009-2012). Seven departments were involved: Physics, Chemistry, Bioengineering, Biochemistry, Computer Science, Mathematics and Material Sciences.

Undergraduate Research

Trained 7 undergraduate students – 4 Physics and 3 Civil Engineering majors. The work resulted into 6 publications in peer reviewed journals and numerous poster presentations.

Trained 5 high school students from Governor School for Science and Mathematics (GSSM) and results reported in 2 papers in peer reviewed journals and a presentation on a poster session at Clemson University.

Lab webpage: <http://compbio.clemson.edu/>

PUBLICATIONS

Refereed Journal Publications

- 1) I Ijaodoro, Y Shao, E Alexov, S Zhao, On generalizing the induced surface charge method to heterogeneous Poisson-Boltzmann models for electrostatic free energy calculation, Journal of Computational Physics, 114452, 2025.
- 2) I Shapovalov, P Rimal, P Poudel, V Lewtas, M Bell, SK Panday, BJ Laight, ...E. Alexov, P. Greer, Quantification and structure–function analysis of calpain-1 and calpain-2 protease subunit interactions, Journal of Biological Chemistry 301 (6), 2025.
- 3) P Poudel, I Shapovalov, SK Panday, K Nouri, PL Davies, PA Greer, E. Alexov, In Silico Screening for Small Molecules to Alter Calpain Proteolysis through Modulating Conformation Changes Induced by Heterodimerization, Journal of Chemical Information and Modeling 65 (11), 5528-5543, 2025.
- 4) AY Chen, SK Panday, K Ri, E Alexov, BR Brooks, A Damjanovic, PKAD-R: curated, redesigned and expanded database of experimental pKa values in proteins, Journal of computational biophysics and chemistry 24 (9), 1189, 2025.
- 5) P Poudel, MA Miteva, E Alexov, Strategies for in Silico Drug Discovery to Modulate Macromolecular Interactions Altered by Mutations, Frontiers in Bioscience-Landmark 30 (4), 26339, 2025.

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- 7) P Rimal, SK Paul, SK Panday, E Alexov, Further Development of SAMPDI-3D: A Machine Learning Method for Predicting Binding Free Energy Changes Caused by Mutations in Either Protein or DNA, *Genes* 16 (1), 101, 2025.
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- 11) S Zhao, IE Ijaodoro, M McGowan, E Alexov, Calculation of electrostatic free energy for the nonlinear Poisson-Boltzmann model based on dimensionless potential, *Journal of Computational Physics* 497, 112634, 2024.
- 12) P Pandey, E Alexov, Most monogenic disorders are caused by mutations altering protein folding free energy, *International Journal of Molecular Sciences* 25 (4), 1963, 2024.
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- 14) P Pandey, S Ghimire, B Wu, E Alexov, On the linkage of thermodynamics and pathogenicity, *Current Opinion in Structural Biology* 80, 102572, 2023.
- 15) N Ancona, A Bastola, E Alexov, PKAD-2: New Entries and Expansion of Functionalities of the Database of Experimentally Measured pKa's of Proteins, *Journal of Computational Biophysics and Chemistry*, 1-10, 2023.
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- 17) S Sun, P Poudel, E Alexov, L Li, Electrostatics in Computational Biophysics and Its Implications for Disease Effects, *International Journal of Molecular Sciences* 23 (18), 10347, 2022.
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