

# CURRICULUM VITAE

Atanu Acharya, PhD

Assistant Professor, Department of Chemistry, Syracuse University, Syracuse, NY

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## EDUCATION AND DEGREES

- 2016 Ph.D. in Chemistry  
Department of Chemistry, University of Southern California, Los Angeles, USA  
Thesis: Photoinduced redox reactions in biologically relevant systems  
Advisor: Prof. Anna I. Krylov
- 2011 M.Sc. in Chemistry  
Department of Chemistry, Indian Institute of Technology Madras (IITM), Chennai, India  
Thesis: Adiabatic and quasi-diabatic potential energy surface of  $H^+ + O_2$  system  
Advisor: Prof. Sanjay Kumar
- 2009 B.Sc. in Chemistry (with honors)  
Department of Chemistry, Jadavpur University, Kolkata, India

## EMPLOYMENT

- 2022 – current Assistant Professor  
Department of Chemistry, Syracuse University, Syracuse, NY, USA

## EXPERIENCES

- 2019 – 2022 Postdoctoral Fellow  
Department of Physics, Georgia Institute of Technology, Atlanta, USA  
Advisor: Prof. James C. Gumbart
- 2017 – 2018 Postdoctoral Associate  
Department of Chemistry, Yale University, New Haven, USA  
Advisor: Prof. Victor S. Batista

## AWARDS AND HONORS

- 2021 Best presentation award from the Molecular BioMedical (MBM) research group seminar series
- 2016 Dissertation Completion Fellowship for excellent research as graduate student
- 2016 Predoctoral scholarship for excellent progress in research as graduate student
- 2015 Dulligan Memorial Award for outstanding graduate research in physical chemistry
- 2015 Travel award for 24<sup>th</sup> winter I-APS conference
- 2014 Best poster award at TCS 2014, CSIR-NCL, Pune, India
- 2011 Best dissertation award for Master thesis from Department of Chemistry, IITM
- 2010 Recipient of Summer Research Fellowship of Indian Academy of Sciences

## TEACHING EXPERIENCES

- CHE 645: Quantum Mechanics in Chemistry Spring 2023
- CHE 400/600: Computational Chemistry and Biochemistry Fall 2022, Fall 2023

### Before Syracuse University

- 2021 School of Physics, Georgia Institute of Technology  
Taught the “Quantum Biology” module of the biophysics graduate course in Fall 2021
- 2011-2013 Department of Chemistry, University of Southern California  
Teaching Assistant for General Chemistry (105 A/B) for six semesters

## MENTORING EXPERIENCES

### Postdoctoral trainees

2023 – curr. Dr. Ronit Sarangi  
2023 – curr. Dr. Sasthi Charan Mandal

### Graduate students

Fall 2022 – curr. Suman Maity, Chemistry

### Undergraduate students

Summer 2023 Micaela Primer, REU student, Chemistry

### Before Syracuse University

2020 Jinchuan Liu and Yupeng Li, Undergraduate students, Georgia Tech  
2017-2018 Subhajyoti Chaudhuri and Peter Dahl, Graduate students, Yale University  
2016 Tirthendu Sen, Graduate student in Krylov group, University of Southern California  
2016 Alina Arslanova, REU student, University of Southern California  
2013 Roman Konoplev-Esgenburg, REU student, University of Southern California  
2013 Bailey Qin, Graduate student in Krylov group, University of Southern California

## PUBLICATIONS

**Google scholar citations: 1006 and h-index: 15 (as of August 1, 2023)**

1. S. Maity and **A. Acharya**; *Many roles of carbohydrates: A computational spotlight on the coronavirus S protein binding.* **ACS Appl. Bio Mater.** 2023. DOI: 10.1021/acsabm.2c01064. [Link To Article](#)
2. Y. Li<sup>1</sup>, **A. Acharya**<sup>1</sup>, L. Yang, J. Liu, E. Tajkhorshid, H. I. Zgurskaya, M. Jackson, and J. C. Gumbart; *Insights into substrate transport and water permeation in the mycobacterial transporter MmpL3.* **Biophys. J.** 2023, 122, 2342-2352, **1<sup>st</sup> authorship shared.** [Link To Article](#)
3. Y. T. Pang<sup>1</sup>, **A. Acharya**<sup>1</sup>, D. L. Lynch, A. Pavlova, J. C. Gumbart; *SARS-CoV-2 spike opening dynamics and energetics reveal the individual roles of glycans and their collective impact.* **Commun. Biol.** 2022, 5, 1170, **1<sup>st</sup> authorship shared.** [Link To Article](#)

### Before Syracuse University

4. C. Stevens, A. N. Pandya, W. Li, Y. Li, J. Mehla, R. Scott, P. Hegde, P. K. Prathipati, **A. Acharya**, J. Liu, J. C. Gumbart, J. North, M. Jackson, H. I. Zgurskaya; *Proton transfer activity of the reconstituted Mycobacterium tuberculosis MmpL3 is modulated by substrate mimics and inhibitors.* Accepted, **Proc. Natl. Acad. Sci.** 2022, 119, e2113963119. [Link To Article](#)  
**Press:** [Phys.org](#), [ThePrint](#), [Hindustan Times](#), and [Times Now](#)
5. B. Yu, M. R. Choudhury, X. Yang, S. L. Benoit, E. Womack, K. V. M. Lyles, **A. Acharya**, A. Kumar, C. Yang, A. Pavlova, M. Zhu, Z. Yuan, J. C. Gumbart, D. W. Boykin, R. J. Maier, Z. Eichenbaum, and B. Wang; *Restoring and enhancing the potency of existing antibiotics against drug-resistant Gram-negative bacteria through the development of potent small-molecule adjuvants.* **ACS Infect. Dis.** 2022, 8, 1491-1508. [Link To Article](#)
6. P. J. Dahl, S. M. Yi, Y. Gu, **A. Acharya**, C. Shippes, J. Neu, J. P. O'Brien, U. N. Morzan, S. Chaudhuri, M. J. Guberman-Pfeffer, D. Vu, S. E. Yalcin, V. S. Batista, and N. S. Malvankar; *A 300-fold conductivity increase in microbial cytochrome nanowires due to temperature-induced restructuring of hydrogen bonding networks.* **Sci. Adv.** 2022, 8, eabm7193. [Link To Article](#)  
**Press:** [ErekAlert](#), [Phys.org](#), [SciTechDaily](#), [ChemEurope](#), [Bioengineer](#), and [Yale News](#)
7. **A. Acharya**, D. Yi, A. Pavlova, V.A. Agarwal, and J. C. Gumbart; *Resolving the hydride transfer pathway in oxidative conversion of proline to pyrrole.* **Biochemistry** 2022, 61, 206-215. [Link To Article](#)

8. [A. Acharya\\*](#), D. L. Lynch, A. Pavlova, Y. T. Pang, and J. C. Gumbart; *ACE2 glycans preferentially interact with SARS-CoV-2 over SARS-CoV*. **Chem. Commun.** 2021, 57, 5949-5952. \*co-corresponding author. [Link To Article](#)
9. A. Pavlova, Z. Zhang, [A. Acharya](#), D. L. Lynch, Y. T. Pang, Z. Mou, J. M. Parks, C. Chipot, and J. C. Gumbart; *Machine learning reveals the critical interactions for SARS-CoV-2 spike protein binding to ACE2*. **J. Phys. Chem. Lett.** 2021, 12, 5494-5502. [Link To Article](#)
10. D. Yi, [A. Acharya](#), J. C. Gumbart, W. Gutekunst, and V. Agarwal; *Gatekeeping ketosynthases dictate initiation of assembly line biosynthesis of pyrrolic polyketides*. **J. Am. Chem. Soc.** 2021, 143, 7617-7622. [Link To Article](#)
11. Z. Zhang, D. Ryoo, C. Balusek, [A. Acharya](#), M. O. Rydmark, D. Linke, and J. C. Gumbart; *Inward-facing glycine residues create sharp turns in  $\beta$ -barrel membrane proteins*. **BBA – Biomembranes** 2021, 1863, 183662. [Link To Article](#)
12. A. Pavlova et al.; *Inhibitor binding influences the protonation states of histidines in SARS-CoV-2 main protease*. **Chem. Sci.** 2021, 12, 1513-1527. [Link To Article](#)
13. [A. Acharya](#) et al.; *Supercomputer-based ensemble docking drug discovery pipeline with application to Covid-19*. **J. Chem. Inf. Model.** 2020, 60, 5832–5852. [Link To Article](#).  
**Press:** [ScienMag](#), [Bioengineer.org](#), [Phys.org](#), [EurekAlert](#), and [Observer](#).
14. S. E. Yalcin, J. P. O'Brien, Y. Gu, K. Reiss, S. M. Yi, R. Jain, V. Srikanth, P. Dahl, W. Huynh, D. Vu, [A. Acharya](#), S. Chaudhuri, T. Varga, V. S. Batista, and N. S. Malvankar; *Electric field stimulates production of highly conductive microbial OmcZ nanowires*. **Nat. Chem. Biol.** 2020, 16, 1136-1142. [Link To Article](#)  
**News and Views, Press:** [Yale press release](#), [Scientific American](#), [Phys.org](#), [ErekAlert](#), [Live Science](#), [Oxford Instruments](#), [NBC-SYFY](#), [American Society of Microbiology](#) (podcast @16:30), [greenreport](#) (italy), [SciTechDaily](#), and [SpaceDaily](#). In [98<sup>th</sup> percentile](#) across all journals.
15. [A. Acharya](#), J. Stockmann, L. Beyer, A. Nabers, J. C. Gumbart, K. Gerwert, and V. S. Batista; *The effect of (-)-epigallocatechin-3-gallate on the amyloid- $\beta$  secondary structure*. **Biophys. J.** 2020, 119, 349-359. [Link To Article](#)
16. K. W. East, J. C. Newton, U. N. Morzan, Y. Narkhede, [A. Acharya](#), E. Skeens, G. Jogl, V. S. Batista, G. Palermo, G. P. Lisi; *Allosteric motions of the CRISPR-Cas9 HNH nuclease probed by NMR and molecular dynamics*. **J. Am. Chem. Soc.**, 2020, 142, 1348-1358. [Link To Article](#)
17. T. Sen, A. V. Mamontova, A. V. Titelmayer, A. M. Shakhov, A. A. Astafiev, [A. Acharya](#), K. A. Lukyanov, A. I. Krylov, and A. M. Bogdanov; *Influence of the first chromophore-forming residue on photobleaching and oxidative photoconversion of EGFP and EYFP*. **Int. J. Mol. Sci.**, 2019, 20, 5229. [Link To Article](#)
18. S. Chaudhuri, [A. Acharya](#), E. T. J. Nibbering, and V. S. Batista; *Regioselective ultrafast photoinduced electron transfer from naphthols to halocarbon solvents*. **J. Phys. Chem. Lett.**, 2019, 10, 2657–2662. [Link To Article](#)
19. J. A. Christensen, B. T. Phelan, S. Chaudhuri, [A. Acharya](#), V. S. Batista, and M. R. Wasielewski; *Phenothiazine radical cation excited states as super-oxidants for energy demanding reactions*. **J. Am. Chem. Soc.**, 2018, 140, 5290-5299. [Link To Article](#)
20. [A. Acharya\\*](#), S. Chaudhuri, and V. S. Batista; *Can TDDFT describe excited electronic states of naphthol photoacids? A closer look with EOM-CCSD*. **J. Chem. Theory Comput.** 2018, 14, 867-876; \* co-corresponding author. [Link To Article](#)
21. [A. Acharya](#), A. M. Bogdanov, B. L. Grigorenko, K. B. Bravaya, A. V. Nemukhin, K. A. Lukyanov, and A. I. Krylov; *Photoinduced chemistry in fluorescent proteins: Curse or blessing?* **Chem. Rev.**, 2017, 117, 758 – 795. [Link To Article](#)
22. P. K. Gurunathan<sup>1</sup>, [A. Acharya](#)<sup>1</sup>, D. Ghosh, D. Kosenkov, I. Kaliman, Y. Shao, A. I. Krylov, and L. V. Slipchenko; *The extension of the effective fragment potential method to macromolecule*. **J. Phys. Chem. B**, 2016, 120, 6562 – 6574; <sup>1</sup>first authorship shared. [Link To Article](#)

23. A. M. Bogdanov<sup>1</sup>, A. Acharya<sup>1</sup>, A. Titelmayer, A. V. Mamontova, K. B. Bravaya, A. B. Kolomeisky, K. A. Lukyanov, and A. I. Krylov; *Turning on and off photoinduced electron transfer in fluorescent proteins by pi-stacking, halide binding, and Tyr145 mutations*. **J. Am. Chem. Soc.**, 2016, 138, 4807 – 4817; <sup>1</sup>first authorship shared. [Link To Article](#) [ACS Live Slide](#)
24. D. Ghosh, A. Acharya, S.C. Tiwari, and A.I. Krylov; *Towards understanding the redox properties of model chromophores from the green fluorescent protein family: An interplay between conjugation, resonance stabilization, and solvent effects*. **J. Phys. Chem. B**, 2012, 116, 12398 – 12405. [Link To Article](#)

## PERSPECTIVE

1. B. Rudshiteyn, A. Acharya, and V. S. Batista; *Is the supporting information the venue for reproducibility and transparency?* **J. Phys. Chem. A** 2017, 121, 968; **J. Phys. Chem. B** 2017, 121, 11425; **J. Phys. Chem. C** 2017, 121, 28212. [Link To Article](#)

## INVITED TALKS

1. *Capturing the role of chemical environments: from electron transfer to virus binding* Department of Chemistry, **Syracuse University**, January 27, 2022
2. *Capturing the role of chemical environments: from electron transfer to virus binding* Department of Chemistry, **University of Alabama at Birmingham**, January 20, 2022
3. *“Capturing the role of chemical environments: from electron transfer to virus binding”* Department of Chemistry, **Texas A&M University**, December 14, 2021
4. *“Role of local environments in chemistry and biochemistry: from electron transfer to virus binding”* **Statistical Mechanics in Chemistry and Biology (SMCB) Seminar Series**, December 4, 2021
5. *“Photoinduced electron transfer from naphthols to Solvents”* **Atlanta Mini-symposium on Theoretical and Computational Chemistry**, October 23, 2021
6. *“Computational techniques in chemistry”* Science department, **Oxford College of Emory University**, February 10, 2021
7. *“Excited-state electron transfer in small molecules and in biology”* **Georgia State University**, July 20, 2018
8. *“Excited-state electron transfer in small molecules and in biology”* **Georgia Institute of Technology**, July 23, 2018

## CONTRIBUTED TALKS

1. *Dynamics and interaction of coronavirus receptor binding domains with glycans*. **ACS National Meeting & Exposition** (San Diego, CA and virtual, Spring 2022)
2. *Resolving the hydride transfer pathway in the oxidative conversion of proline to pyrrole*. **ACS National Meeting & Exposition** (San Diego, CA and virtual, Spring 2022)
3. *ACE2 glycans preferentially interact with SARS-CoV-2 over SARS-CoV*. **Pacificchem 2021** (Honolulu, HI and virtual)
4. *ACE2 glycans preferentially interact with SARS-CoV-2 over SARS-CoV*. **Southeastern Regional Meeting of ACS** (Birmingham, AL, Fall 2021)
5. *ACE2 glycans preferentially interact with SARS-CoV-2 over SARS-CoV*. **Molecular BioMedical (MBM) seminar series** (Georgia Tech, 2021)
6. *Differences in the interactions of receptor binding domains of SARS-CoV-2 and SARS-CoV with ACE2 glycans*. **ACS National Meeting & Exposition** (Atlanta, GA and virtual, Fall 2021)
7. *Resolving the hydride transfer pathway in Bmp3-catalyzed pyrrole biosynthesis*. **ACS National Meeting & Exposition** (Atlanta, GA and virtual, Fall 2021)

8. *Exploring photoinduced electron transfer leading to "oxidative redding" in fluorescent proteins.* **ACS National Meeting & Exposition** (San Diego, CA, Spring 2016)

## **POSTER PRESENTATIONS**

1. *Distinct states of MmpL3 in lipid transport across the mycobacterial inner membrane.* **ACS National Meeting & Exposition** (San Diego, CA and virtual, Spring 2022)
2. *Distinct Differences in the Interactions of Receptor Binding Domains of SARS-CoV-2 and SARS-CoV with Human ACE2.* **BPS Annual Meeting** (Virtual, 2021)
3. *The effect of (-)-epigallocatechin-3-gallate on the A $\beta$  secondary structure.* **BPS Annual Meeting** (San Diego, CA, 2020)
4. *Ring-modulated excited state electron transfer in naphthol photoacids.* **Gordon Research Conference: Electron Donor-Acceptor Interactions** (Newport, RI, 2018)
5. *Molecular level understanding of photo-bleaching and oxidative-redding via electron transfer in fluorescent proteins.* **ACS National Meeting & Exposition** (Philadelphia, PA, 2016)
6. *Exploring photo-induced electron transfer leading to "oxidative redding" in fluorescent proteins.* **Gordon Research Conference: Molecular Interactions and Dynamics** (Easton, MA, 2016)
7. *Turning on and off photoinduced electron transfer in fluorescent proteins by  $\pi$ -stacking, halide binding and TYR145 mutations.* **Gordon Research Conference: Photochemistry** (Easton, MA, 2015)
8. *Exploring oxidative redding of proteins from GFP family: A gateway step approach.* **24th Winter I-APS Conference** (Sarasota, FL, 2015)
9. *Exploring oxidative redding of proteins from GFP family: A gateway step approach.* **Theoretical Chemistry Symposium**, CSIR-National Chemical Laboratory (Pune, India, 2014)
10. *Exploring oxidative redding of proteins from GFP family: A gateway step approach.* **The American Conference on Theoretical Chemistry** (Telluride, CO, 2014)
11. *Redox properties of green fluorescent proteins and their chromophores.* **54th Sanibel symposium** (St. Simons Island, GA, 2014)
12. *Adiabatic and quasi-diabatic potential energy surface of H<sup>+</sup>+CO system.* **Theoretical Chemistry Symposium**, Indian Institute of Technology Kanpur (Kanpur, India, 2010)

## **WORKSHOP ATTENDED**

2013 Software summer school at Virginia Tech by Innovation Institute for Computational Chemistry and Materials Modeling (S2I2C2M2)

## **GRANTS**

Currently funded

08/2023 – 07/2028                      NIH R35GM150874                      \$1,862,500 (\$1,250,000 direct)                      PI  
Investigation of Long-Range Charge Transfer and Excited State Processes in Biochemical Systems

## **COMPUTATIONAL RESOURCES GRANTS**

1. XSEDE start-up grant (2017-2019) as a PI (CHE170024) for the project "Towards understanding and enhancing electrical conductivity of bacterial pili protein"
2. ANTON2 allocations (2019) with Prof. Victor S Batista for the project "Towards understanding electron transport pathways of conductive geobacter pili and design principle for enhancement of their conductivity"

## **SKILLS/EXPERIENCE**

- Software packages: Q-Chem, IQmol, Gaussian, Gaussview, ORCA, NAMD, VMD, Autodock, and Maestro
- Scripting languages: Python and Tcl
- Multiscale modelling: QM/MM calculations and effective fragment potential
- Electronic structure calculations: DFT, TDDFT, CCSD, and EOM-CCSD
- Molecular dynamics (MD) simulations, enhanced sampling techniques – targeted MD, steered MD, and Gaussian-accelerated MD.
- Charge transfer
- Excited-state processes

## **SERVICES**

### Student Committees

- PhD thesis committee: Hedyeh Zamani, Yuchen Jin
- MS thesis committee: Britnie Carpentier
- 2<sup>nd</sup> year student committee: Warren Kincaid

### Panel Member

- Two review panels in 2023 for National Science Foundation (NSF).

### Peer-review service

- ACS Omega
- Biophysical Journal
- Chemical Communications
- Computer Physics Communications
- Chemical Science
- Journal of Chemical Information and Modeling
- Journal of Chemical Theory and Computation
- Journal of Physical Chemistry A/B/C/Letters
- Nature Communications
- Organic and Biomolecular Chemistry
- Physical Chemistry Chemical Physics

### Other service

- Judged Clayton county public school (CCPS) regional science & engineering fair in 2022
- Proctored United States National Chemistry Olympiad (USNCO) competition in 2021
- Judged posters in undergraduate research symposium at Georgia Tech in 2019