# **RATUL CHOWDHURY**, Ph. D

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## ✦ EDUCATION

**The Pennsylvania State University (Costas Maranas Lab)**
Ph.D. in Chemical Engineering + Minor in Computational Sciences — Dec/19
Thesis title: *Computational redesign of channel proteins, enzymes, and antibodies*

**Jadavpur University, Kolkata, India**
Bachelor of Science in Chemical Engineering — May/13

## ✦ RESEARCH INTERESTS

- Deep Learning on protein sequence, structure, and functional landscapes
- Activity and specificity engineering of proteins
- Protein interaction with proteins and non-proteins
- Protein-based biomaterials
- Drug-discovery in context of human proteome
- Structure-guided metabolic modeling, pathway design, and strain engineering

## ✦ PROFESSIONAL EXPERIENCE

Assistant Professor, Department of Chemical and Biological Engineering — Jul/22-present
Iowa State University, Ames, IA.

Postdoctoral Fellow, Laboratory of Systems Pharmacology — Jan/20-Jun/22
Harvard Medical School, Boston, MA.
*Advisors:* Prof. Peter Sorger

Graduate Research Assistant, Department of Chemical Engineering — Jul/13-Dec/19
The Pennsylvania State University, University Park, PA.
*Advisor:* Prof. Costas D. Maranas

Graduate Teaching Assistant, Department of Chemical Engineering — Jan/17-May/17
The Pennsylvania State University, University Park, PA.

Research Intern, Mechanobiology Institute — Apr/12-Jul/12
National University of Singapore, 5A Engineering Drive 1, Singapore.
*REU Mentor:* Prof. P. Kanchanawong

Research Intern, Molecular Reproduction, Development and Genetics — Apr/11-Jul/11
Indian Institute of Science, Biological Science Bldg., Karnataka 560012, India
*REU Mentor:* Prof. R. Dighe

## ✦ HONORS AND AWARDS

- **Selected Speaker at SynBYSS** Synthetic Biology Young Speaker Series 2022 (EBRC - **https://ebrc.org/**) /2021
- **Invited Guest Editor** for Special Issue in *Frontiers in Biotech. & Bioengineering* (**Issue**) /2021
- **Alumni Spotlight** | Penn State University 2020 / Distinguished Alumni Series (**Article link**) /2020
- Cover article for Nature Materials, Volume 19, Issue 3 /2020
- AIChE Separations Divisions, Dibakar Bhattacharyya Outstanding Graduate Researcher Award /2019
- Enzyme Engineering Conference XXV Conference Travel Award /2019

- Biochemical & Molecular Engineering XXI Conference Graduate Award /2019
- **NAMS Outstanding Young Membrane Researcher Award** (North American Membrane Society) /2019
- Graduate Research Travel Award for NAMS 2019 conference – Pittsburgh /2019
- **Brown Graduate Award** (Best Graduate Symposium Poster Award – Penn State) /2018
- **Ward Graduate Award** (Best Graduate Student Paper of the Year Award *for* PoreDesigner -*Nature Comm*) /2018
- Best **Poster Award** (**Gordon Research Conference**, Membranes, New Hampshire) /2018
- Best **Oral Presentation Award** (**Gordon Research Seminar**, Membranes, New Hampshire) /2018
- MDPI **Feature Paper** – OptMAVEn-2.0 published in MDPI journal *Antibodies*, Vol. 7 /2018
- Best **Oral Presentation in Rational Protein Engineering** (AIChE Annual Meeting, Minnesota) /2017
- Summer Research Fellowship, Mechanobiology Lab, National University of Singapore /2012
- **Distinguished Undergraduate Attendee** at Thirteenth Marcel Grossmann Meeting, Stockholm /2012
- Summer Research Fellowship, **Department of Science and Technology**, Govt. of India /2011
- **Best Presenter Award** and Summer Cosmology Workshop Invitation (*IUCAA, Pune, India*) /2010
- Kishore Vaigyanik Protsahan Yojana (**KVPY**) – highest undergraduate research award from Govt. of India /2010

## ✦ PUBLICATIONS

Published/ Accepted/ Under review (* *Equal contribution*)

- *Antiviral efficacy and mechanisms of plant-derived polyphenols for inactivation of Tulane virus, a surrogate for human norovirus.* ***ASM***
  C Oh*, R Chowdhury*, …, M Kumar. [Green chemistry | Water Purification] /2022

- *Computational prediction of the effect of amino acid changes on the binding affinity between SARS-CoV-2 spike and human ACE2 receptor.* ***PNAS***
  C Chen, VS Boorla, R Chowdhury, …, CD Maranas. [Protein Structure | SARS CoV-2] /2021

- *Foldamer-based ultrapermeable and highly selective artificial aquaporins that exclude protons.* ***Nature Nanotechnology***
  A Roy, J Shen, H Joshi, R Chowdhury, ..., M Kumar. [Nature-inspired | Biophysics] /2021

- *De novo design of high-affinity antibody variable regions (scFv) against the SARS-CoV-2 spike protein.* (Under Review: ***Proteins***)
  VS Boorla, R Chowdhury*, …, JJ Gray, CD Maranas. [Protein Structure | SARS CoV-2] /2021

- *Recombination and lineage-specific mutations led to the emergence of SARS-CoV-2.* ***Genome Medicine***
  JAP Galindo, I Filip, R Chowdhury, …, R Rabadan. [Protein Structure | SARS CoV-2] /2021

- *Computational biophysical characterization of the SARS-CoV-2 spike protein binding with the ACE2 receptor and implications for infectivity.* ***Computational Structural Biotechnology Journal***
  R Chowdhury*, VS Boorla, and CD Maranas. [Protein Structure | SARS CoV-2] /2020

- *Rapid fabrication of precise high-throughput filters from membrane protein nanosheets*. ***Nature Materials*** ** featured article*
  YM Tu, W Song, …, R Chowdhury, ..., M Kumar. [Nature-inspired | Biophysics] /2020

- *IPRO+/- Computational protein design tool allowing for insertions and deletions.* ***Structure – Cell Press***
  R Chowdhury, …, CD Maranas. [Enzyme Engineering | Protein Function] /2020

- *Engineering sensitivity and specificity of AraC-based biosensors responsive to triacetic acid lactone and orsellinic acid.* ***Protein Engineering Design and Selection***
  Z Wang, A Doshi, R Chowdhury, …, PC Cirino. [Biosensor | Protein Function] /2020

- *From directed evolution to computational enzyme engineering—A review*.
  ***AIChE Journal***
  R Chowdhury and CD Maranas. [Enzyme Engineering] /2019

- *Artificial water channels enable fast and selective water permeation through water-wire networks*. ***Nature Nanotechnology***
  W Song, H Joshi, R Chowdhury, ..., M Kumar. [Nature-inspired | Biophysics] /2019

- *Directed evolution reveals the functional sequence space of an adenylation domain specificity code*. ***ACS Chemical Biology***
  K Throckmorton, V Vinnik, R Chowdhury, ..., BF Pfleger. [Enzyme Engineering | Protein Function] /2019

- *7-log virus removal in a simple functionalized sandfilter*.
  ***Environmental Science & Technology***
  L Samineni, B Xiong, R Chowdhury, …, M Kumar. [Green Chemistry | Water Purification] /2019

- *PoreDesigner for tuning solute selectivity in a robust and highly permeable outer membrane pore*.
  ***Nature Communications***
  R Chowdhury, T Ren, …, CD Maranas. [Channel Protein | Separations] /2018

- *OptMAVEn-2.0: De novo design of variable antibody regions against targeted antigen epitopes*.
  ***Antibodies – MDPI*** ** featured article*
  R Chowdhury, MF Allan, and CD Maranas. [Immunology | Protein Structure] /2018

- *Highly active C8-acyl-ACP thioesterase variant isolated by a synthetic selection strategy*.
  ***ACS Synthetic Biology***
  N Hernandez, R Lai, R Chowdhury, ..., BF Pfleger. [Enzyme Engineering | Protein Function] /2018

- *Facile affinity maturation of antibody variable domains using natural diversity mutagenesis*. ***Frontiers in Immunology***
  KE Tiller, R Chowdhury, …, P Tessier. [Immunology | Protein Structure] /2017

- *Using gene essentiality and synthetic lethality information to correct yeast and CHO cell genome-scale models*. ***Metabolites – MDPI***
  R Chowdhury, A Chowdhury, CD Maranas. [Metabolic Modeling | Bio-networks] /2015

- *Conversion of slaughterhouse and poultry farm animal fats and wastes to biodiesel: Parametric sensitivity and fuel quality assessment*. ***Renewable and Sustainable Energy Reviews***
  R Chakraborty, AK Gupta, R Chowdhury. [Biofuel | Energy] /2013

- *Application of ANFIS model to optimize the photocatalytic degradation of chlorhexidine digluconate*.
  ***Royal Society of Chemistry – Advances***
  S Sarkar, R Chowdhury, ..., C Bhattacherjee. [Process Optimization | Neural Network] /2013

- *Interacting generalized cosmic Chaplygin gas in loop quantum cosmology: A singularity free universe*. ***International Journal of Theoretical Physics***
  R Chowdhury, and P Rudra. [Cosmology | Thermodynamics] /2012

- *Influence of gauss-bonnet coupling parameter on the thermodynamic properties of Einstein-Gauss-Bonnet and Einstein-Yang-Mills-Gauss-Bonnet black holes*. ***International Journal of Theoretical Physics***
  R Chowdhury, R Biswas, …, S Chakraborty. [Cosmology | Thermodynamics] /2012

✦ PATENT

- US20190329189A1. Title: ANGSTROM-SCALE "SEPARATIONS BY DESIGN" USING PRECISION BIOMIMETIC MEMBRANE. (Penn State Invention Disclosure No. 2018-4764).
  [patents.google.com/patent/US20190329189A1/en]

## ✦ SELECTED MEDIA COVERAGE

- *ScienceMag* | Solving a Natural Riddle of Water Filtration (Article link) /2021
- *UT Austin Research Headlines* | Solving a Natural Riddle of Water Filtration (Article link) /2021
- *Alumni Spotlight* | Penn State University 2020 / Distinguished Alumni Series (Article link) /2020
- *Nature Nanotechnology News and Views* | A new type of artificial water channels. *Nature Nanotechnology* /2020
- *ScienceDaily* | Protein pores packed in polymers make super-efficient filtration membranes (Article link) /2020
- *Chemical & Engineering News* (C&En) | Filter from tropical tree seeds purges viruses from water (Article link) /2019
- *AIChE Separations Division Outstanding Researchers of 2019* | (Article link) /2019
- *North American Membrane Society Student Fellows 2019* | (Article link) /2019
- *UT Austin Research Headlines* | Bio-inspired new water filtration method (Article link) /2019
- *Penn State Chemical Engineering News* | Building better membranes (Article link) /2019
- *Penn State Research Headlines* | PoreDesigner process improves water treatment, bio-separations (Article link) /2018
- *Phys.Org* | PoreDesigner improves protein channel design for water treatment (Article link) /2018
- *Penn State Chemical Engineering News* | Research symposium – graduate student achievements (Article link) /2018

## ✦ INVITED TALKS

*Single-sequence protein structure prediction and enzyme engineering*
**Manifold Bio**. Waltham, MA. /2022

*Consequences of single-sequence protein structure prediction.*
**Statistical Thermodynamics & Molecular Simulations** Seminar Series. Yale University. CT. /2022

*Single-sequence protein structure prediction and antimicrobial peptide design*
Dept. of Environmental Engineering. **University of Illinois-Urbana Champaign.** IL. /2022

*Single-sequence protein structure prediction using deep learning*
Dept. of Environmental Engineering. **University of Texas at Austin.** TX. /2021

*Protein design in the world of deep learning*.
**Nested Therapeutics**. Boston, MA. /2021

*The future of protein engineering in the presence of AlphaFold2*.
**Zymergen**. Emeryville, CA. /2021

*Novel protein engineering tool for predicting insertions and deletions along with substitutions.*
**Enzyme Engineering Conference XXV**. Whistler, British Columbia, Canada. /2019

P*rotein engineering for Separations*.
Popular lecture series **Research Unplugged**. Schlow Library. Penn State. /2018

*New paradigms in protein design and precise aqueous separation devices*.
**Bioinformatics and Genomics Annual Retreat**. *Huck Institute of Life Sciences*. Penn State. /2018

## ✦ SELECTED ORAL AND POSTER PRESENTATIONS (speaker/ presenter)

*Structure-guided phylogeny of human kinome*. **CCSP-NIH**. Virtual. USA. /2022

*PoreDesigner for precise tuning of OmpF for high solute selectivity*
**STARTech Conference (NASA)**, TX. USA. /2018

*PoreDesigner for engineering protein channels for precise angstrom scale bio-separations*
**Gordon Research Conference**, Membranes, NH. USA. **Best poster awardee* /2018

*Biomimetic pore design for precise angstrom scale bio-separations*
**Gordon Research Conference**, Membranes, NH. USA. **Best talk awardee* /2018

*PoreDesigner for engineering protein channels for precise angstrom scale bio-separations*
**Graduate Symposium** Penn State University. PA. USA. **Best poster awardee* /2018

*Computational substrate specificity switching of sorghum phenylalanine-ammonia lyase*
**Center for Bio-Innovation**, DOE Annual Meeting, TN. USA. /2018

*Redesign of E. coli water channel protein OmpF using Iterative Protein Redesign and Optimization Suite*
**AIChE Annual Meeting**, MN. USA. **Best talk awardee* /2017

I*nteracting Generalized Cosmic Chaplygin Gas in Loop Quantum Cosmology*
**Marcel Grossmann Meeting**, Stockholm. Sweden. **UG best poster awardee* /2012

## ✦ TEACHING AND MENTORING

### During Ph.D.

- **Teaching Assistant**. Design of Chemical Plants (CHE470),
  Department of Chemical Engineering, Penn State /2018
- **Graduate online teaching certificate** for future faculty (OL2050), World Campus Online
  Faculty Development. Penn State World Campus – *Certificate* /2019
- **Several** REU and graduate students mentored:
  (a) describing project goals, (b) assigning deliverables, (c) setting up shared GitHub repositories
  for version control, (d) analyzing data, and (e) drafting manuscripts. /2016-19

## ✦ SERVICE

### Reviewer Activity

*Nature Communications, Nature Scientific Data, Nature Scientific Reports, PNAS, Science, Cell Systems, Cell – Structure, PloS Computational Biology, ACS | Langmuir, Frontiers in Immunology, Metabolic Engineering, and Frontiers in Bioengineering and Biotechnology (Guest Editor: Special issue 2022 – Advances in Protein Structure, Function, and Design).*