

# Rohit Goswami

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*“An unproblematic state is a state without creative thought. Its other name is Death.”  
– David Deutsch*

## Personal Data

Name Rohit Goswami  
Date Of Birth 10.08.1995  
Birthplace Brookhaven, New York, United States of America

## Work Experience

- 2019–PRESENT **Faculty of Physical Sciences, University of Iceland**, Graduate Researcher.  
I am working with Prof. Hannes Jónsson on Bayesian analysis and machine learning for *ab-initio* quantum chemistry.
- 2019–PRESENT **Department of Chemistry, Indian Institute Of Technology, Kanpur**, Senior Project Associate.  
I am affiliated to the Femtolab under the project “Femtosecond Laser Approaches to Quantum Information and Quantum Computation”
- 2018–2019 **Department of Chemical Engineering, Indian Institute Of Technology, Kanpur**, Project Associate.  
I was associated with the Computational Nanoscience group. Over the course of two centrally funded projects, “Nucleation On Nanostructured Surfaces Computer Simulation Studies (SPO/DST/CHE/2017294)” and “Advanced Computation Research and Education (SPO/MHRD/CC/20130176)”:
- I worked on the implementation of an enhanced version of the CHILL (CHILL+) algorithm for tracking ice types.
  - Designed a linear discriminant analysis technique for near-surface ice structure determination which is undergoing rigorous testing
  - Implemented a graph based network connectivity model for ice structures
  - Spearheaded the development of High Performance GPU accelerated molecular dynamics simulation analysis tools
  - Worked on the determination of optimal GPU cluster configurations
  - Designed and administered academic outreach websites

## Education

- 2019–PRESENT **Graduate studies, University of Iceland, Reykjavik, Iceland.**  
Current GPA: 9.0
- 2014–2018 **B.Tech. Chemical Engineering, Harcourt Butler Technical University, Kanpur, India.**  
First Division (PROJECT: Gas Sweetening Plant Design)
- 2011–2013 **Intermediate (AISSCE), Delhi Public School Kalyanpur, Kanpur, India.**  
87.2% Central Board of Secondary Education (CBSE)
- 2009–2011 **High School (AISSE), Delhi Public School Kalyanpur, Kanpur, India.**  
9.8 Cumulative Grade Point Average (CGPA) in Central Board of Secondary Education (CBSE)

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## Voluntary Positions

- JULY-AUGUST 2020 **Water, Chemicals and more with Computers for Chemistry (WC3m)**, *Wave Learning Festival*, Co-Teacher.  
15 hour long summer course for high school students and undergrads on the basics of computational chemistry.
- JUNE-JULY 2020 **Online Data Carpentry Workshop**, *SADiLaR, South Africa*, Lead Instructor.  
Taught the basics of R, OpenRefine, and some data wrangling to graduate students in the social sciences over three days.
- JUNE-JULY 2020 **Data Carpentry Ecology Workshop**, *Biotech Partners*, Leading Instructor.  
Taught the basics of Python and assisted with shell lessons for high school students over three days, with a follow up mentoring program.
- 2020-2021 **Executive Student Council**, *American Institute of Chemical Engineers*, Publications Webmaster.  
Am tasked with managing the publications committee web resources.
- MAY 2020 **Helper**, *CodeRefinery Mega Workshop*.
- APRIL-MAY 2020 **CS106A - Code in Place**, *Stanford University*, Section Leader (TA).  
As part of the special COVID-19 code-in-place initiative, I worked as a section leader (teaching assistant). The course covered the fundamentals of computer programming using Python and was built off the first half of CS106A. Also moderated and participated in an AMA session on "Machine Learning for the Physical Sciences" and taught a workshop for the other section leaders entitled "Functional Python Packaging with Nix"
- 2019-PRESENT **IEEE P1940**, *IEEE Standards Committee*, Working group member.  
Am actively engaged in working with stake holders in industry and academia to create a collection of standard profiles that define integration of authentication services with ISO 8583 used for financial transactions.
- 2019-PRESENT **R Novice Inflammation**, *The Carpentries*, Maintainer.  
As a maintainer for the Software Carpentries lesson on R, I work with the community to make sure that lessons stay up-to-date, accurate, functional and cohesive.
- 2019-PRESENT **CarpentryCon 2020**, *The Carpentries*, Program Committee co-chair & Website subcommittee member.  
Working for an international conference with diverse leads from across the world, as part of the program committee I reached out to keynote speakers and managed the overall schedule. Wrote content with the website subcommittee and also contributed due to my web development expertise.
- 2019-PRESENT **Univ.ai**, *Earth2Orbit Analytix Private Limited*, Teaching Fellow and Developer.  
Tested course-content and developed interactive labs to work with an online cohort of students. Am presently teaching labs and mentoring small batches. I also work with the front and backend teams to facilitate workflows including shopify stores and NodeJS authentication systems.
- 2018-2019 **Animal Welfare Group**, *Indian Institute of Technology Kanpur*, Member and Web-developer.  
Have worked with student bodies to rescue and care for local animals. Also designed and maintain a site with ReactJS to enhance knowledge dissemination.

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## Undergraduate Experience

### Internships

- 2017-2018 **Dr. Debojit Chakrabarty**, *Keva Fragrances Ltd, Mumbai*, R&D Industrial Intern.  
Modeling complex multi-component perfumes in a predictive method via experimental and theoretical considerations. In collaboration with Prof. Rajdip Bandyopadhyaya of the ChemE Dept. at IIT Bombay.
- SUMMER 2017 **Prof. Sibasish Ghosh**, *The Institute of Mathematical Sciences, Chennai*, Visiting Scholar.  
Discussed computational techniques for the simulation and understanding of quantum tomography.
- SUMMER 2017 **Prof. Nisanth Nair**, *Indian Institute Of Technology Kanpur*, SURGE Scholar.  
An exploratory project to understand and deal with bottlenecks in computational chemistry, the major objectives were to investigate hybridization of existing code via OpenMP and MPI.

POSTER: Development of Computational Tools for Free Energy Calculations of Chemical Reactions

SUMMER 2016 **Dr. Rajarshi Chakrabarti**, *Indian Institute Of Technology Bombay*, Research Intern.

Retooled a server with ArchLinux and also simulated patchy colloids (Janus Particles).

PROJECT REPORT: Computational Survey of Coarse Grained Soft Matter Molecular Dynamics Simulations

### Volunteer Work

2017–2018 **ChemE Herald**, *Harcourt Butler Technical University, Kanpur*, Editor-in-Chief.

Inaugurated and managed an interdisciplinary technical newsletter.

2017–2018 **HBTU-MUN 2018**, Secretary General.

Designed a ReactJS based static website, with Trello backed user registration, also performed outreach pre-events to raise awareness and participation, in addition to overseeing the working of the executive board.

2016–2017 **HBTU-MUN 2017**, Executive Board Chairperson.

Designed a Jekyll based static website and ensured adherence to standard MUN rules as Chairperson.

2014–2016 **The Curiosity Magazine**, *Harcourt Butler Technical University, Kanpur*, Editor-in-Chief.

Managed a diverse team of student content writers and also later typeset a spin-off multi-lingual newsletter in X<sub>Y</sub>L<sup>A</sup>T<sub>E</sub>X.

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## Technical Skills

### Programming Languages

EXPERIENCED C++, Python, R, FORTRAN, Shell (zsh, bash), OpenMP, OpenMPI, Tcl, CSS, JS, HTML, Sass, C

FAMILIAR Ruby, Julia, Java, Haskell, Matlab, Golang, ReactJS, Node, CUDA

### Projects

EXPERIENCED d-SEAMS, Android (Cyanogen, LineageOS, AOSP), Web-Design (static), ArchLinux

FAMILIAR Linux Kernel (Android)

### Simulation Projects

EXPERIENCED ESPResSo (Extensible Simulation Package for Research on Soft matter), LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator), OVITO, AiiDA (Automated Interactive Infrastructure and Database for Computational Science)

FAMILIAR OpenFOAM, GROMACS (Groningen Machine for Chemical Simulations), VMD (Visual Molecular Dynamics)

### Tools

EXPERIENCED X<sub>Y</sub>L<sup>A</sup>T<sub>E</sub>X, pandoc, Git (version control), tmux, ssh, Vim, Sublime Text Editor 3, gnuplot, gadfly, bspwm (tiling window manager), babun, MATLAB (matrix laboratory), Continuous Integration Services (Wercker, Travis CI, Semaphore CI), docker

FAMILIAR AWS (Amazon Web Services), moltemplate, jekyll, middleman, grunt, gulp, Frameworks (Bourbon, Skeleton, neat) Markup Languages (Textile, HAML, Jade(pug))

### Opensource Contributions

CREATED PixN ROM & Kernel (AOSP based rom for the Xperia Z5)  
HaoZeke's LineageOS

MANTAINED Xperia Z5 LineageOS (14.\*)

### Opensource Projects Created

d-SEAMS An open-source, community supported engine for the analysis of molecular dynamics trajectories (co-creator)

ZENYODA	Pandoc based, tup driven stand-alone multi format (revealJS, beamer etc.) presentation system with static site generation.	DOCUYODA	A document generation system based on pandoc and latexmk driven by gulp with yaml configuration and easy templating.
STARDOCK	Docker compose based containerized self-updating setup for media hosting, with traefik for reverse proxying. Includes music, ebook and video acquisition and management.	PYQTNUMSIM	A Qt interface for verbose numerical methods assignments.
GRIMOIRE	Metalsmith and webpack based open source educational experiment with a strong focus on readability, equations and references.	RGOSWAMI.ME	A hugo-blog template meant to be used with Emacs orgmode

## Affiliations & Accolades

### Memberships

2014–PRESENT	<b>OSA (Optical Society of America)</b> , Student Member → Early Career Member (2018).
2015–PRESENT	<b>AIChE (American Institute Of Chemical Engineers)</b> , Student Member → Young Professional (2018).
2015–PRESENT	<b>APS (American Physical Society)</b> , Student Undergraduate Member → Early Career Member (2019).
2015–PRESENT	<b>IEEE (Institute of Electrical and Electronics Engineers)</b> , Student Member → Early Career Member (2018).
2015–PRESENT	<b>IOP (Institute of Physics)</b> , Student Member (2018) → Member (2019).
2006–PRESENT	<b>World Taekwondo</b> , Red Belt.
2009–PRESENT	<b>XDA Developers</b> , Senior Member.
2019–PRESENT	<b>AAAI (Association for the Advancement of Artificial Intelligence)</b> , Professional Member.
2019–PRESENT	<b>ACM (Association for Computing Machinery)</b> , Professional Member. Also part of the SIGHPC (Special Interest Group for High Performance Computing) & SIGHPC-Education
2019–PRESENT	<b>ASAPBio (Accelerating Science and Publication in biology)</b> , Ambassador.
2019–PRESENT	<b>ICHEME (Institute of Chemical Engineers)</b> , Associate Member.
2019–PRESENT	<b>IICHE (Indian Institute of Chemical Engineers)</b> , Life Associate Member.
2019–PRESENT	<b>IEEE IAS (Industrial Applications Society)</b> , Member.
2019–PRESENT	<b>IEI (The Institution of Engineers [India])</b> , Associate Member.
2019–PRESENT	<b>InRaSS (Indian Radio Science Society)</b> , Student Member.
2019–PRESENT	<b>OSI (Open Source Initiative)</b> , Individual Member.
2019–PRESENT	<b>OSI (Optical Society of India)</b> , Life Fellow.
2019–PRESENT	<b>SPIE (Society of Photo-Optical Instrumentation Engineers)</b> , Early Career Professional.
2019–PRESENT	<b>The Carpentries</b> , Certified Instructor.
2019–PRESENT	<b>URSI (Union Radio-Scientifique Internationale)</b> , Corresponding Member.
2020–PRESENT	<b>Heterodox Academy</b> , Graduate Affiliate Member.
2020–PRESENT	<b>IGDORE (Institute for Globally Distributed Open Research and Education)</b> , Researcher-in-training.
2020–PRESENT	<b>COS (Center for Open Sciences)</b> , Ambassador.
2020–PRESENT	<b>ims (Institute of Mathematical Statistics)</b> , Student Member.
2020–PRESENT	<b>Bernoulli Society</b> , Student Member.
2020–PRESENT	<b>RSS (Royal Statistical Society)</b> , E-Student Member.

2020–PRESENT **Computing at School**, Member.

### Awards

DECEMBER 2016 **Photonics-2016**, *Indian Institute Of Technology Kanpur*, Springer Best Student Paper Award, Nonlinear-Optics Session.

2014–2015 **IITG Zephyr Creative Writing**, *Indian Institute Of Technology Guwahati*, First Prize.

2014–2015 **Antaragni IITK-MUN GA-DISEC**, *Indian Institute Of Technology Kanpur*, Best Speaker.

### Reviews

2018–PRESENT **Journal Of Open Source Software**, Reviewer.

2019–PRESENT **PeerJ - Life & Environment**, Reviewer.

2019–PRESENT **PeerJ - Computer Science**, Reviewer.

2019–PRESENT **PeerJ - Organic Chemistry**, Reviewer.

2019–PRESENT **PLOS ONE**, Reviewer.

2020–PRESENT **APS Physical Review Letters**, Reviewer.

2020–PRESENT **SPIE Journal of Micro/Nanolithography, MEMS, and MOEMS**, Reviewer.

2020–PRESENT **IOP - Machine Learning: Science and Technology**, Reviewer.

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## Publications

### JOURNALS

Rohit Goswami, Amrita Goswami, and Jayant Kumar Singh. “d-SEAMS: Deferred Structural Elucidation Analysis for Molecular Simulations.” In: *Journal of Chemical Information and Modeling* (Mar. 2020). ISSN: 1549-9596. DOI: 10.1021/acs.jcim.0c00031. URL: <https://doi.org/10.1021/acs.jcim.0c00031>.

Rohit Goswami. “Don’t Pull Punches in Peer Review.” In: *Nature* 574 (Oct. 8, 2019), pp. 176–176. DOI: 10.1038/d41586-019-03024-2. URL: [/articles/d41586-019-03024-2](https://doi.org/10.1038/d41586-019-03024-2) (visited on 10/09/2019).

Prerna, Rohit Goswami, Atanu K. Metya, S. V. Shevkunov, and Jayant K. Singh. “Study of Ice Nucleation on Silver Iodide Surface with Defects.” In: *Molecular Physics* (Aug. 25, 2019), pp. 1–13. ISSN: 0026-8976, 1362-3028. DOI: 10.1080/00268976.2019.1657599.

### CONFERENCE PROCEEDINGS

R. Goswami and D. Goswami. “Quantum Distributed Computing with Shaped Laser Pulses.” In: *13th International Conference on Fiber Optics and Photonics* (2016). DOI: 10.1364/photonics.2016.w4c.3.

R. Goswami, A. Goswami, and D. Goswami. “Space Filling Curves: Heuristics For Semi Classical Lasing Computations.” In: *2019 URSI Asia-Pacific Radio Science Conference (AP-RASC)*. Mar. 2019, pp. 1–4. DOI: 10.23919/URSIAP-RASC.2019.8738612.

### PREPRINTS

Nairhita Samanta, Rohit Goswami, and Rajarshi Chakrabarti. *Diffusion of self-propelled Janus tracer in polymeric environment*. 2017. arXiv: 1704.06207.

Rohit Goswami, Amrita Goswami, and Jayant K. Singh. *d-SEAMS: Deferred Structural Elucidation Analysis for Molecular Simulations*. 2019. arXiv: arXiv:1909.09830.

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## Conference Records

### Posters

MARCH 2020 **Ultrafast Insights for Predictive Fragrance Compounding**, *ACS Spring 2020 National Meeting*, R. Goswami, A. K. Rawat, D. Chakrabarty, and D. Goswami, Accepted.

DECEMBER 2019 **Qubit Network Barriers to Deep Learning**, *IEEE WRAP-2019*, R. Goswami, A. Goswami, and D. Goswami.



- MARCH 2019 **Space Filling Curves: Heuristics For Semi Classical Lasing Computations**, *URSI Asia-Pacific Radio Science Conference (AP-RASC 2019)*, R. Goswami, A. Goswami, and D. Goswami.
- DECEMBER 2018 **FDTD Numerical Computations for Ultrafast Non-linear Optics**, *Photonics-2018*, R. Goswami, A. Goswami, and D. Goswami.
- Oral Presentations
- AUGUST 2020 **Reproducible Environments with the Nix Packaging System**, *CarpentryCon 2020*, R. Goswami and A. Goswami.
- JULY 2020 **LFortran: Interactive LLVM-based Fortran Compiler for Modern Architectures**, *FortranCon 2020*, O. Čertík, N. Maan, A. Pandey, M. Curcic, P. Brady, Z. Jibben, N. Carlson, R. Goswami, A. Shahmoradi and A. Markus, Presented by Ondřej.
- DECEMBER 2019 **Process Safety in terms of Latent Dirichlet Allocations**, *72nd Annual Session of the Indian Institute of Chemical Engineers, CHEMCON-2019*, R. Goswami, Accepted.
- OCTOBER 2019 **Semi-Supervised Approaches to Ultrafast Optimal Control Theory**, *43rd Symposium of the Optical Society of India, International Conference on Optics & Electro-Optics*, R. Goswami, A. Goswami and D. Goswami.
- DECEMBER 2016 **Quantum Distributed Computing with Shaped Laser Pulses**, *13th International Conference on Fiber Optics and Photonics*, R. Goswami and D. Goswami.

## Workshops and Schools

- OCTOBER 2020 **Computational materials discovery of unconventional magnets**, *EPFL, Lausanne, Switzerland*, The proposed workshop aims to bring together researchers both from theory and experiments working on different aspects of the field to present the latest advancements and to discuss the efforts required to expedite the discovery of new unconventional magnetic materials., Accepted.
- OCTOBER 2020 **ESPresSo and Python: Versatile Tools for Soft Matter Research**, *CECAM School*, The school focuses on the introduction of particle-based coarse-grained Molecular Dynamics simulation techniques for Hard and Soft Matter systems with the freely available software package ESPResSo. Includes lectures and hands-on sessions., Accepted.
- SEPTEMBER 2020 **(Machine) learning how to coarse-grain**, *CECAM and TRR146 Virtual Event*, The purpose of this workshop will be to discuss the current state of the art, some of the challenges that the community is facing in furthering the penetration of ML models in CG simulations, and future perspectives., Accepted.
- SEPTEMBER 2020 **Gaussian Process and Uncertainty Quantification Summer School**, *University of Sheffield, UK*, The Gaussian Process Summer Schools are a series of schools and workshops aimed at researchers who want to understand and use Gaussian process models, both in theory and practice., Accepted.
- JULY 2020 **AiiDA Virtual Tutorial**, *EPFL, Lausanne, Switzerland*, A four day online in-depth tutorial by core and plugin developers covering the nuances of reproducible workflows for AiiDA with example Quantum ESPRESSO calculations on Quantum Mobile virtual machines..
- JUNE 2020 **Mathematical Methods of Modern Statistics 2**, *CIRM Virtual Event*, A five day online event from the Centre International de Rencontres Mathématiques on recent statistical advances relating to the analysis of high dimensional data from frequentist and Bayesian perspectives..
- MAY 2020 **ALCF Computational Performance Workshop**, *Online*, A three day workshop on the hardware and software improvements organized by Argonne Leadership Computing Facility..
- OCTOBER 2019 **TriangleSCI 2019**, *Invited to the Triangle Scholarly Communication Institute*, A week long fully-funded incubator to discuss actionable goals towards Bringing Equity and Diversity to Peer Review. This was undertaken as part of the larger discussion on Equity in Scholarly Communications, **declined to attend**.
- MAY-JUNE 2019 **Artificial Intelligence, E & ICT Academy**, *IIT Kanpur*, A four week course on AI foundations culminating in a time-series prediction project.
- JUNE 2019 **AI Foundations Certificate Course**, *univ.ai*, A summer school taught in-person by faculty from Harvard and UCLA, culminating in a computer vision and neural network based identification project.

JULY 2019 **Rare Events Summer School**, *Indian Institute of Science, Bangalore*, A short course consisting of lectures and hands-on sessions by experts in the field, organized by Prof. Baron Peters.

### Short Courses

SEPTEMBER 23<sup>rd</sup> 2019 **Surface Area and Porous Material Characterization**, *Dept. of ChemE, IIT Kanpur*, An intensive day long course on the basics of experimental classification and DFT methods for pore distribution by Dr. Martin Thomas from Anton-Paar.

SEPTEMBER 21<sup>st</sup> 2019 **OpenACC GPU Bootcamp**, *Chemistry Department, IIT Kanpur*, Day long programming session and discussion covering the acceleration of Institute in-house code facilitated by a Senior Nvidia Solution Architect (Mr. Bharatkumar) and Prof. Debabrata Goswami.

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## Certifications

### Coursera

MARCH 2020 **Deep Learning Specialization**, *deeplearning.ai*, 99.5%.

The specialization can be verified by ID Q3DLMZJ42TR. This signifies the completion of the following five courses:

- Neural Networks and Deep Learning - **100.0%**
- Improving Deep Neural Networks: Hyperparameter tuning, Regularization and Optimization - **99.2%**
- Structuring Machine Learning Projects - **98.3%**
- Convolutional Neural Networks - **100.0%**
- Sequence Models - **100.0%**

### NPTEL Courses

JAN-APR 2019 **Graph Theory**, *IISER Pune*, 55%.

License: NPTEL19MA13S21460067

AUG-SEP 2018 **Computational Chemistry and Classical Molecular Dynamics**, *IIT Bombay, Elite*, 77%.

License: NPTEL18CS13S21440127

AUG-SEP 2018 **Introduction to Parallel Programming in OpenMP**, *IIT Madras*, 40%.

License: NPTEL18CS55S11440122

JAN-APR 2018 **Quantum Computing**, *IIT Kanpur, Elite*, 65%.

License: NPTEL18CY07S4480024

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## Graduate Coursework

“Due to COVID-19, grading varies from P/F to a 10 point scale.” (Note)

SUMMER 2020 **Seminar on Machine Learning**, *University of Iceland*, Computer Science Dept., Pass.

Research seminar.

**Presentation:** How Powerful are Graph Neural Networks?

SUMMER 2020 **Statistics, science and COVID-19**, *University of Iceland*, Health Sciences Institute, 10.

Course covering “Statistical Rethinking” by Richard McElreath as well as the COVID-19 model of the University.

**Project:** Icelandic Housing Analysis

SPRING 2020 **Probabilistic Data Analysis**, *University of Turku, Finland*, Turku Data Science group.

Research seminar based on “Bayesian Data Analysis” by Andrew Gelman, John Carlin, Hal Stern, David Dunson, Aki Vehtari, and Donald Rubin

**Presentation:** Markov Chain Simulations

SPRING 2020 **Applied data analysis**, *University of Iceland*, Mathematics and Applied Statistics Dept., 10.

Course covering “Introduction to Statistical Learning An Introduction to Statistical Learning with Applications in R” by Gareth James, Daniela Witten, Trevor Hastie and Robert Tibshirani

**Project:** Icelandic Housing Analysis

- SPRING 2020 **Applied data analysis - Project**, *University of Iceland*, Mathematics and Applied Statistics Dept., Pass.  
Extra credit course  
**Project:** Molecular Dynamics Trajectory Analysis
- SPRING 2020 **Machine Learning**, *University of Iceland*, Computer Science Dept., Pass.  
An overview of some of the main concepts, techniques and algorithms in machine learning. Supervised learning, unsupervised learning and reinforcement learning. Data preprocessing and data visualization. Model evaluation and model selection. Linear regression, nearest neighbors, support vector machines and decision trees. Deep learning. Cluster analysis, the k-means and EM algorithms. TD-learning, Q-learning.  
**Project:** Toxic Comment Classification (Grade 9/10)
- SPRING 2020 **Software Quality Management**, *University of Iceland*, Pass.  
Metrics and models: Tools for managing software quality and its improvement. Quality Assurance: standards. Software Quality assurance activities. Quality assurance infrastructure and progress control. Software quality in Agile development.  
**Presentation:** Scrum (Grade 10/10)
- SPRING 2020 **Introduction to Pattern Recognition**, *University of Iceland*, Electrical Engineering Dept., 8.  
Course covering “Elements of Statistical Learning: Data Mining, Inference, and Prediction” by Trevor Hastie, Robert Tibshirani, and Jerome Friedman along with “Pattern Recognition and Machine Learning” by Christopher Bishop.  
**Project:** Predicting Molecular Properties