Mohammad Amin Sadeghi

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Summary

- PhD in Chemical Engineering with a focus on modeling, simulation, and data analytics.
- 10+ years of experience in modeling & simulation, machine learning, and software development.
- Strong project management skills with track record of leading and contributing to cross-functional teams.

Relevant Experience

Al Computational Developer

2024 - Present

Computational Materials Engineering, CanmetMATERIALS – Natural Resources Canada

- Developed a long short term memory (LSTM) time series model to predict Li-ion battery degradation from impedance spectroscopy (EIS) measurements. (NumPyro, PyTorch)
- Designed an active learning end-to-end battery cycling workflow for automated data acquisition, analysis, and model retraining using Bayesian optimization. (NumPyro, JAX)
- Developed a Python interface for automated control and data acquisition from BioLogic potentiostats.

Postdoctoral Fellow 2023 - 2024

Department of Materials Science and Engineering, University of Toronto

- Developed AutoEIS, a Python package for automated analysis of EIS data using genetic algorithms and Bayesian inference. (NumPyro, Julia, JAX)
- Designed, implemented and deployed an EIS processing and visualization dashboard, improving processing efficiency and enabling real-time insights. (Streamlit, Nginx)
- Designed, implemented and deployed a parallelized workflow to collect, process and analyze large-scale EIS datasets on Compute Canada HPC clusters. (SLURM, Shell, MPIRE)

Postdoctoral Fellow 2019 - 2023

Department of Chemical Engineering, University of Waterloo

- Developed a physics-informed convolutional neural network (CNN) to compute the tortuosity of voxel images, up to 1000x faster than physics-based solvers, e.g., FEM, LBM, etc. (PyTorch)
- Implemented a distributed data pipeline to generate a large-scale dataset to train a physics-informed CNN for tortuosity estimation. (Dask, Ray)
- Implemented a convolutional autoencoder to simulate Li-ion battery discharge, 10x faster than COMSOL, to enhance automated screening of electrode microstructures. (TensorFlow, COMSOL)
- Developed reduced order digital twins for various electrochemical systems (e.g., hydrogen fuel cells, electrolyzers) to accelerate in-silico material screening. (SciPy Stack, OpenPNM, PoreSpy)
- Led a team of 10+ developers through the software development lifecycle, enhancing code quality through rigorous code reviews and streamlining deployment processes by implementing CI/CD pipelines. Maintained and deployed the team's online resources on GitHub and AWS.

Research Intern Fall 2018

Object Research Systems (ORS)

• Developed a plugin for Dragonfly¹ to extract pore networks from 3D images of porous materials. (PyQt)

• Learned GUI development using Qt from scratch and delivered a production-quality plugin within 2 months, leading to Dragonfly's market expansion from medical imaging to rock sciences.

Research Assistant 2015 – 2019

Department of Chemical Engineering, McGill University

- Developed a reduced order model for HBr flow batteries; enabling 100x more throughut for optimizing the microstructure while maintaining accuracy. (Python, OpenPNM)
- Developed OpenPNM, a Python package for reduced order modeling of transport in porous media, providing up to 1000x speedup over FEM, LBM, etc. with minimal loss of accuracy.
- Developed PoreSpy, a Python package for image processing of porous media, providing a comprehensive suite of tools for image segmentation, analysis, and visualization.
- Designed and implemented distributed CI/CD pipelines for OpenPNM and PoreSpy, reducing testing time by 80%, leading to more frequent releases and higher code quality.

Research Assistant 2012 – 2015

Department of Chemical Engineering, Sharif University of Technology

- Developed a multiphysics CFD model using COMSOL to simulate reactive flow in catalytic converters, exploring the interplay between cell shape and performance.
- Utilized MATLAB LiveLink API to automate COMSOL model development, creating a fully automated workflow for optimizing CO2/NOx removal in catalytic converters.

Skills

Technical Skills

- Parallel/GPU Programming: Working knowledge of OpenMP, MPI, CUDA, Numba, CuPy for parallel/GPU computing; and Dask, Ray for scalable data processing and model training.
- Image Processing & Visualization: Working knowledge of Scikit-Image, OpenCV. Proficient in data visualization with Matplotlib, Plotly, Seaborn, and ParaView.
- Data Science & Analysis: Proficient in NumPy, SciPy, Pandas, Scikit-Learn. Familiar with databases (SQL, NoSQL) e.g., MySQL, MongoDB, and big data technologies like Apache Spark.
- Cloud Technologies: Working knowledge of using and deploying on cloud services e.g., Google Cloud and AWS. Experience with SLURM scheduling in HPC clusters.
- Programming & Software Development: Working knowledge of version control (Git, Perforce), debugging, and testing. Proficient in Python, C/C++, Julia, MATLAB. Experience with full-stack development using HTML/CSS/JavaScript, and frameworks e.g., Django and Flask. Good understanding of object-oriented programming, design patterns, data structures, and algorithms. Working knowledge of software testing, CI/CD pipelines, and containerization (Docker, Kubernetes).
- Machine Learning & Al: Working knowledge of PyTorch, JAX, TensorFlow. Experienced in building and tuning large-scale, distributed machine learning models.

¹ Scientific image processing software developed by ORS (acquired by Comet)

Advanced Knowledge

- Mathematical & Computational Modeling: Proficient in scientific computing, solving differential equations using FEM, FVM, FDM. Familiar with the Lattice Boltzmann method (LBM). Working knowledge of linear, nonlinear, and stochastic optimization techniques. Working knowledge of Bayesian inference and probabilistic programming.
- Machine Learning Techniques: Working knowledge of supervised and unsupervised learning. Working knowledge of deep learning methods, e.g., convolutional and recurrent neural networks. Familiar with reinforcement learning. Working knowledge of data cleaning, feature engineering, and working with large datasets. Working knowledge of model reduction techniques e.g., PCA, UMAP, etc. Working knowledge of physics-informed machine learning, e.g., physics-informed neural networks, and neural operators.
- Engineering & Simulation: Deep understanding of thermodynamics, fluid mechanics, transport phenomena, and reaction kinetics. Working knowledge of technical drawing and simulation software, e.g., COMSOL Multiphysics, AutoCAD, and Aspen HYSYS.

Soft Skills

Project Management

- Led the development of popular open-source libraries, managing a team of over 10 developers and successfully delivering major releases.
- Managed multiple cross-functional projects concurrently, consistently meeting deadlines and milestones.
- Supervised and mentored undergrad/grad students, leading to successful outcomes, e.g., publications.

Community Engagement

- Actively engaged with the user community to address issues and feature requests for various opensource projects, significantly growing user base and satisfaction.
- Led workshops, tutorials, and coding clubs to promote open-source development and foster collaboration.

• Technical Communication

- Secured ongoing funding for the development of OpenPNM and PoreSpy through effective communication with non-technical stakeholders and funding agencies.
- Authored and co-authored over 20 peer-reviewed journal articles and conference papers.
- Presented research findings at more than 20 international conferences and workshops.

Open-Source Software

OpenPNM (400+ stars, 350+ citations)

- Python library for performing pore network modeling of porous media.
- Led development of the second and third major releases.

PoreSpy (250+ stars, 250+ citations)

- Python library for characterizing and analyzing 2D/3D images of porous materials.
- Led development of the second major release.

AutoEIS (20+ stars, under review at JOSS)

- Python library for automated analysis of electrochemical impedance spectroscopy (EIS) data.
- Led development of the first major release.

Tortuosity.jl (repo public, but not yet released)

• Julia package (+ Python wrapper) for computing tortuosity from voxel images.

TauNet (repo private until paper published)

- Python package for rapid estimation of tortuosity from voxel images using physics-informed CNNs.
- Demonstrated up to 1000x speedup over the SOTA¹ physics-based solvers on various datasets.

Education

McGill University | Montreal, Canada

2015 - 2019

- Ph.D. in Chemical Engineering
- Thesis: Role of electrode microstructure on battery performance using computational modeling

Sharif University of Technology | Tehran, Iran

2012 - 2015

- M.S. in Chemical Engineering
- Thesis: CFD-aided modeling and shape optimization of CO2/NOx catalytic converters

Sharif University of Technology | Tehran, Iran

2008 - 2012

- B.S. in Chemical Engineering
- Graduating Dean's Honors List

Leadership

University of Toronto

2017 - 2023

Co-Supervisor

Sara Shi: Predicting remaining useful life of Li-ion batteries using impedance spectroscopy (PhD, 2023)

University of Waterloo

2017 - 2023

Co-Supervisor

- Ricky Fan: Estimation of Tortuosity of Large Images using Domain Decomposition (BSc, 2023)
- Sam Ly: Modeling of the State of Lithiation in Li-Ion Batteries via Autoencoders (MSc, 2023)
- Mike McKague: Parallelized Network Extraction from Voxel Images using Medial Axis (PhD, 2022)
- Niloo Misaghian: Pore Network Modeling of Zinc-Air Batteries (PhD, 2022)
- Mike McKague: Pore Network Modeling of Physical Adsorption in Porous Media (MSc, 2020)

Sharif Computer-Aided Chemical Engineering Contest (SC₃¹)

2012 - 2015

Founder, President (3x)

- Chaired the scientific committee responsible for designing problem sets.
- Secured sponsorship and oversaw executive tasks.
- Grew the competition from 15 to 300+ participants in 3 years.

Manuscripts Under Review/Preparation

• Sadeghi, M.A., Ly, S., and Gostick, J.T. (2024) TauNet: An interpretable deep learning framework for rapid estimation of tortuosity from voxel images. To be submitted to *npj Computational Materials*.

¹ State of the Art

¹ A nationwide programming competition for chemical engineering students in Iran

• Sadeghi, M.A., and Gostick, J.T. (2024) Estimation of tortuosity of tomograms using a GPU-accelerated transient Laplace solver. To be submitted to *Computers & Geosciences*.

Peer-Reviewed Publications

- Ly, S., Sadeghi, M.A., Misaghian, N., Fathiannasab, H., and Gostick, J. (2024) Rapid prediction of particle-scale state-of-lithiation in Li-ion battery microstructures using convolutional neural networks. Applied Energy, 360, p.122803.
- Bell, E., Morris, D., **Sadeghi, M.A.**, and Gostick, J. (2024) BEaTmap: Simplified Rigorous BET Analysis of Isothermal Adsorption Data. *Journal of Open Research Software*, 12(1).
- Sadeghi, M.A., Khan, Z.A., Agnaou, M., Hu, L., Litster, Gostick, J. (2023) Predicting PEMFC performance from a volumetric image of catalyst layer structure using pore network modeling. *Applied Energy*, 353, p.122004.
- Misaghian, N., Sadeghi, M.A., and Gostick, J.T. (2023) Utilizing pore network modeling for performance analysis of multi-layer electrodes in vanadium redox flow batteries. *Journal of The Electrochemical* Society, 170 (7), 070520.
- van Gorp, R., van der Heijden, M., **Sadeghi, M.A.**, Gostick, J., Forner-Cuenca, A. (2023) Bottom-up design of porous electrode by combining a genetic algorithm and a pore network model. *Chemical Engineering Journal*, p.139947.
- Misaghian, N., Sadeghi, M.A., Roberts, E., Gostick, J. (2022) Investigating the role of the triple-phase boundary in zinc-air cathodes using pore network modeling. *Journal of The Electrochemical Society*, 169(10), p.100549.
- Amini, K., **Sadeghi, M.A.**, Pritzker, M., Gostick, J. (2022) Porous electrodes in redox flow batteries. *Encyclopedia of Energy Storage*; Cabeza, L. F., Ed.; Elsevier: Oxford, 2022; pp 466-479.
- McKague, M., Fathiannasab, H., Agnaou, M., Sadeghi, M.A., and Gostick, J. (2022) Extending pore networks
 to include electrical double layer effects in micropores for capacitive deionization. Desalination, 535,
 p.115784.
- Misaghian, N., Agnaou, M., Sadeghi, M.A., Fathiannasab, H., Hadji, I., and Gostick, J. (2022) Prediction of diffusional conductance in network models using convolutional neural networks. Computers & Geosciences, 162, p.105086.
- van der Heijden, M., Van Gorp, R., **Sadeghi, M.A.**, Gostick, J., and Forner-Cuenca, A. (2022) Assessing the versatility of network modeling to simulate flow battery performance. *Journal of The Electrochemical Society*, 169(4), p.040505.
- Khan, Z., Agnaou, M., Sadeghi, M.A., Elkamel, A., Gostick, J. (2021) Pore network modelling of galvanostatic discharge behavior of lithium-ion battery cathodes. Journal of The Electrochemical Society, 168(7), 070534.
- Pourali, M., Esfahani, J.A., Sadeghi, M.A., Kim, K.C., Gostick, J. (2021) Simulation of steam reforming in a
 catalytic micro-reactor using an analytical approach. International Journal of Hydrogen Energy, 46(44),
 pp.22763-22776.

- Agnaou, M., Sadeghi, M.A., Tranter, T.G., Gostick, J. (2020) Modeling transport of charged species in pore networks: solution of the Nernst-Planck equations coupled with fluid flow. Computers & Geosciences, p.104505.
- Sadeghi, M.A., Agnaou, M., Barralet, J., Gostick, J. (2020) Dispersion in pore networks: A comparison of common models and alternative approaches. *Journal of Contaminant Hydrology*, 228, p.103578.
- Tavakolian, M., Wiebe, H., **Sadeghi, M.A.**, and van de Ven, T.G. (2019) Dye removal using hairy nanocellulose: experimental and theoretical investigations. *ACS Applied Materials & Interfaces*, 12(4), pp.5040-5049.
- Zhang, Z., **Sadeghi, M.A.**, Jervis, R., Ye, S., Gostick, J., Barralet, J.E., Merle, G. (2019) Tailoring carbon nanotube microsphere architectures with controlled porosity. *Advanced Functional Materials*, 29(42), p.1903983.
- Sadeghi, M.A., Agnaou, M., Kok, M., Aghighi, M., Gostick, J. (2019) Exploring the impact of microstructure on flow battery performance using a multiphysics network model. *Journal of The Electrochemical Society*, 166(10), p.A2121.
- Gostick, J.T., Khan, Z.A., Tranter, T.G., Kok, M.D., Agnaou, M., **Sadeghi, M.**, and Jervis, R. (2019) PoreSpy: a python toolkit for quantitative analysis of porous media images. *The Journal of Open Source Software*, 4(37), p.1296.
- Kok, M.D., Jervis, R., Tranter, T.G., **Sadeghi, M.A.**, Brett, D.J.L, Shearing, P.R., Gostick, J. (2019) Mass transfer in fibrous media with varying anisotropy for flow battery electrodes. *Chemical Engineering Science*, 196, pp.104-115.
- Sadeghi, M., Aghighi, M., Barralet, J., Gostick, J. (2017) Pore network modeling of transport in hierarchical porous particles: the effects of microstructure. *Chemical Engineering Journal*, 330, pp.1002-1011.
- Sadeghi, M., Salami, H., Taghikhani, V., Robert, M.A. (2015) A comprehensive study on CO2 solubility in brine: Thermodynamic and neural network modeling. *Fluid Phase Equilibria*, 403, pp.153-159.

Conference Presentations

- McKague, M.G., Sadeghi, M.A. and Gostick, J., May. (2024) Pore network modelling of a lithium-ion battery cathode as a tool for microstructure optimization. In 245th ECS Meeting (May 26-30, 2024).
- van der Heijden, M., **Sadeghi, M.A.**, Gostick, J., Forner-Cuenca, A. (2023) Starting from the bottom: Coupling a genetic algorithm and a network model for porous electrode optimization. 15th Annual Interpore Meeting, Edinburgh, UK.
- Sadeghi, M.A., Khan, Z.A., Agnaou, M., Gostick, J. (2022) Predicting the performance of PEMFC by just looking at an image! 4th Annual CREATE and Use Hydrogen, Calgary, Canada.
- Sadeghi, M.A., Khan, Z.A., Agnaou, M., Gostick, J. (2022) Pore-scale modeling of multiphysics and multiphase transport in porous electrode components. Gordon Research Conference, Fuel Cells, Smithfield, United States.
- Sadeghi, M.A., Gostick, J. (2022) From pydns to DNS.jl: How we translated our Python package to Julia. 4th Annual Canadian Research Software Conference (CRSC), Montreal, Canada.

- Sadeghi, M.A., Gostick, J. (2022) DNS.jl: a finite-difference transient diffusion solver for tomography images. 4th Annual Canadian Research Software Conference (CRSC), Montreal, Canada.
- Misaghian, N., Agnaou, M., Sadeghi, A., Fathiannasab, H., Gostick, J. (2021) Utilizing deep learning to
 predict diffusional conductance in network models. 71st Canadian Chemical Engineering Conference,
 Montreal, Canada.
- Sadeghi, M.A., Gostick, J. (2021) How we automated our software development cycle using GitHub Actions. 3rd Annual Canadian Research Software Conference (CRSC), Virtual.
- Sadeghi, M.A., Gostick, J. (2021) Rapid estimation of effective diffusivity using a GPU-accelerated transient finite-difference solver. 3rd Annual Canadian Research Software Conference (CRSC), Virtual.
- Sadeghi, M.A., Khan, Z.A., Agnaou, M., Litster, S., Gostick, J. (2021) Multiphysics multiscale modeling of fuel cell catalyst layer: a pore network modeling study. 13th Annual Interpore Meeting, Virtual.
- Aggarwal, C., Sadeghi, M.A., Monte, E., Lowman, J., Gostick, J., Abukhdeir, N.M. (2021) Determination of characteristic transport coeff. of porous media: A diffuse interface approach. 13th Annual Interpore Meeting, Virtual.
- McKague, M., Fathiannasab, H., Agnaou, M., Sadeghi, M.A. and Gostick, J. (2021) Application of Helmholtz electric double layer theory in a pore network model for capacitive deionization. 13th Annual Interpore Meeting, Virtual.
- v/d Heijden, M., van Gorp, R., Szendrei, G., **Sadeghi, A.**, Gostick, J., Broneman, Z., Forner-Cuenca, A. (2021) Towards bottom-up design of porous electrode micro-structures: Coupling genetic algorithms with pore network modeling of redox flow battery electrodes. 13th Annual Interpore Meeting, Virtual.
- Agnaou, M., Sadeghi, M.A., Gostick, J.T. (2019) Simulation of multiphysics processes: A pore network modeling approach for ions transport. 2nd Annual Canadian Research Software Conference (CRSC), Montreal, Canada.
- Wiebe, H., Tavakolian, M., **Sadeghi, M.A.**, van de Ven, T.G.M. (2019) Dye removal using hairy nanocellulose. Quebec Center for Advanced Materials, Student Symposium, Montreal, Canada.
- Sadeghi, M.A., Barralet, J., Gostick, J.T. (2018) Nanoscale digital reconstruction of the fuel cell catalyst layer and measurement of eff. properties. 68th Canadian Chemical Engineering Conference, Toronto, Canada.
- Sadeghi, M.A., Barralet, J., Gostick, J. T. (2018) Modeling of dispersion in porous media: derivation of accurate pore network models. 68th Canadian Chemical Engineering Conference, Toronto, Canada.
- Sadeghi, M.A., Barralet, J., Gostick, J. T. (2018) Pore network reconstruction and simulation of the fuel cell catalyst layer. 234th Meeting of The Electrochemical Society, Cancun, Mexico.
- Agnaou, M., Sadeghi, A., Gostick, J. (2018) Multiphysics simulation using OpenPNM: A highly accurate transient dispersion solver. 1st Annual Canadian Research Software Conference (CRSC), Ottawa, Canada.
- Sadeghi, M.A., Barralet, J., Gostick, J. T. (2018) Investigating structure-performance of catalyst layers with network modeling. Gordon Research Conference: Fuel Cells, Smithfield, United States.

- Sadeghi, M.A., Barralet, J., Gostick, J. T. (2018) The impact of electrode pore structure on redox flow battery performance. 10th Annual Interpore Meeting, New Orleans, USA.
- Zhang, Z., Sadeghi, M.A., Gostick, J.T., Barralet, J. (2018) Oxide-anchored, carbide-supported Pt nanoparticles for oxygen reduction reaction. Materials Research Society Spring Meeting & Exhibit, Phoenix, USA.
- Zhang, Z., Sadeghi, M.A., Gostick, J.T., Barralet, J. (2018) Core-shell structured carbide catalysts for oxygen reduction reaction. 8th Electrochemical Society Montreal Student Chapter Symposium, Montreal, Canada.
- Zhang, Z., **Sadeghi, M.A.**, Gostick, J.T., Barralet, J. (2018) Carbide core-shell structures for oxygen reduction reaction. 4th International NanoTech and NanoScience Conference & Exhibition, Paris, France.
- Sadeghi, M.A., Aghighi, M., Barralet, J., Gostick, J.T. (2017) Hierarchical materials to the rescue, or how to use hierarchy of porosity to maximize catalytic activity. 67th Canadian Chemical Engineering Conference, Edmonton, Canada.
- Sadeghi, M.A., Aghighi, M., Gostick, J.T. (2017) The interplay between pore structure and electrode performance: a pore-network modeling study. 67th Canadian Chemical Engineering Conference, Edmonton, Canada.
- Sadeghi, M.A., Aghighi, M., Barralet, J., Gostick, J.T. (2017) Modelling diffusion and reaction in hierarchical porous media with OpenPNM. 9th Annual Interpore Meeting, Delft, Netherlands.
- Sadeghi, M.A., Aghighi, M., Barralet, J., Gostick, J.T. (2016) Pore-scale modeling of transport in a catalyst particle with a hierarchy of porosity. 66th Canadian Chemical Engineering Conference, Quebec City, Canada.
- Sadeghi, M.A., Salami, H., Taghikhani, V. (2012) Modeling of CO2 solubility in brine by using neural networks. 5th EAGE International Conference and Exhibition on Geosciences, Saint Petersburg, Russia.

Awards

1 st prize, Best Oral Presentation 4 th Annual CREATE and Use Hydrogen Conference	2022
3rd prize, Best Poster Award 3 rd Annual Canadian Research Software Conference	2021
1 st prize, Best Poster Award 2 nd Annual Canadian Research Software Conference	2019
1 st prize, Best Poster Award 1 st Annual Canadian Research Software Conference	2018
2 nd prize, Three Minute Thesis (3MT) Canadian Society for Chemical Engineers	2017
Graduate Excellence Fellowship McGill University	2016
McGill Engineering International Tuition Award McGill University	2015
Scholarship for Summer Internship TÜM, NanoSystems Initiative Munich	2014
2 nd prize, Best BSc Thesis Award Iranian Institute of Chemical Engineers	2013
International Travel Grant 5 th EAGE International Conference on Geosciences	2012
Professional Service	

Professional Service

Journal/Conference Reviewer

- Reviewed submissions for the 5th Annual Research Software Engineers Conference (SeptembRSE)
- Peer reviewed articles for prominent journals including Angewandte Chemie, Journal of Power Sources,
 Advances in Water Resources, Transport in Porous Media, Journal of Petroleum Science and Engineering,
 The Journal of Open Source Software

 2019 now

Student Society Member | McGill University

2018 - 2019

• Designed the first prototype of the Chemical Engineering Graduate Student Society website.

IT Officer | McGill University

2018

• Developed an online polling platform for People's Choice award in Chemical Engineering Research Day, enhancing participant engagement.

Scientific Committee Member | McGill University

2018

• Evaluated student posters for the Summer Undergraduate Research in Engineering competition.

Workshop Instructor | Sharif University of Technology

2018

• Conducted workshops on MATLAB 101, Writing Effective Resumes and Statements of Purpose, and Succeeding in TOEFL and GRE Exams.

Student Society Member | Sharif University of Technology

2012 - 2015

• Served as a columnist for the Chemical Engineering Student Society weekly newsletter.

Teaching Experience

Sessional Lecturer | University of Waterloo

Summer 2023

• CHEE 614 Capillary and Transport Phenomena in Porous Media*1

Guest Lecturer | McGill University

Fall 2018

CHEE 662 Computational Methods*

Teaching Assistant | McGill University

2015 - 2019

CHEE 662 Computational Methods* (Fall 2017-18)

- CHEE 641 Chemical Reaction Engineering* (Winter 2018)
- CHEE 440 Process Modeling (Winter 2016-18)
- CHEE 390 Computational Methods (Fall 2016)

Teaching Assistant | Sharif University of Technology

2012 - 2015

- CHEE 662 Computational Methods* (Fall 2017-18)
- CHEE 912 Process Modeling (Winter 2014)
- CHEE 323 Computational Methods (Winter 2012 & Fall 2014)
- CHEE 925 Heat Transfer (Winter 2013)
- CHEE 211 Fluid Mechanics (Fall 2013)
- CHEE 267 Advanced Numerical Methods* (Fall 2013)

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¹ Courses marked with an asterisk (*) are graduate-level.