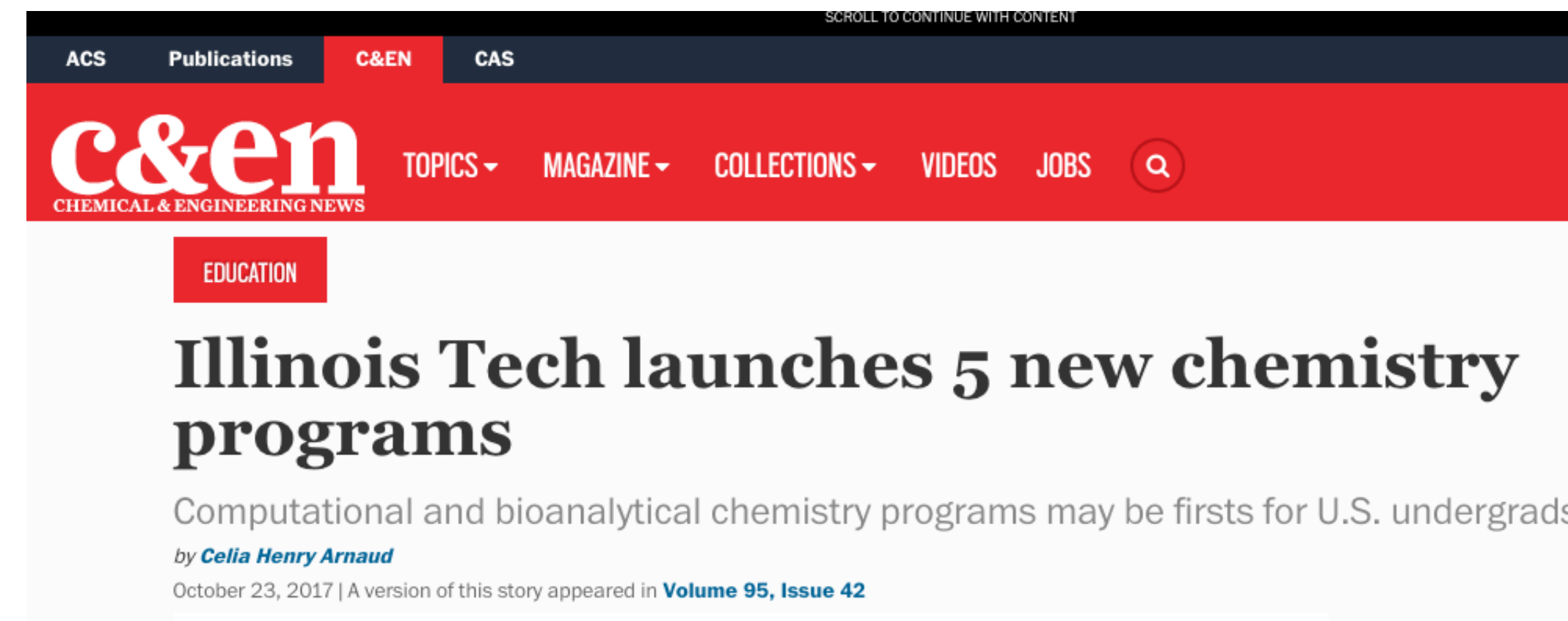


8/26/2024

- Welcome
- Syllabus
- Introductions
- Google Drive Folder Link Setup
- Exercise 1: Introduction to Google Colab

History



- 2004: I attended a workshop on molecular modeling at the beginning of my Ph.D., helping me get off to a quick start
- 2017: Illinois Tech launches five specialized chemistry programs
- 2020: I taught Chem 456 for the first time. It starts in a computer lab and moves online due to the pandemic.
- 2021: In the summer, I organized an online workshop and ran a small session of Chem 456. Examples could be run on a virtual machine.
- 2022: In the Spring, I work with four students to run the workshop in Colombia. We migrate the labs to Google Colab. I teach this class in the Fall.

Syllabus

<https://daveminh.github.io/Chem456-2024F/>

Introductions

About me: work

Biographical

Professional History

2020 – present	Robert E. Frey, Jr. Endowed Faculty in Chemistry , Illinois Institute of Technology (Illinois Tech), Chicago, IL
2019 – present	Associate Professor (tenured), Department of Chemistry, Illinois Tech
2018 – present	Associate Director , Center for Interdisciplinary Scientific Computation, Illinois Tech
2013 – 2019	Assistant Professor (tenure-track), Department of Chemistry, Illinois Tech
2011 – 2013	Postdoctoral Research Associate , Duke University, Durham, NC
2009 – 2011	Director's Postdoctoral Fellow , Argonne National Laboratory, Argonne, IL
2007 – 2009	Postdoctoral Trainee , National Institutes of Health, Bethesda, MD

Education

2004 – 2007	Ph.D. in Physical Chemistry , University of California, San Diego. Thesis Title: Free Energy Reconstruction from Irreversible Single-Molecule Pulling Experiments. Recipient of Molecular Biophysics Training Grant and Aguoron Kamen and Kaplan Fellowship.
2000 – 2003	B.A. in Chemistry , University of California, Berkeley. Recipient of Chancellor's Scholarship (Berkeley's most prestigious scholarship) and National Merit Scholarship.

Awards

2020	College of Letters and Science Nominee, Michael J. Graf IIT Teaching and Advising Innovation Award.
2019	40 under 40 Chicago Scientists. Selected by Halo Cures.
2019	Sigma Xi Junior Faculty Award, in recognition of Outstanding Accomplishments in Research and Scholarship. Awarded by the Illinois Tech chapter of the scientific research honor society, Sigma Xi.
2018	College of Science Dean's Excellence Award in Research, at the Junior Level
2012	OpenMM Visiting Scholar (at Stanford)
2009 – 2011	Director's Postdoctoral Fellowship
2007 – 2009	Postdoctoral Intramural Research Training Award
2005 – 2007	NIH Molecular Biophysics Training Grant
2004 – 2005	Aguoron Kamen and Kaplan Fellowship
2000 – 2003	UC Berkeley Chancellor's Scholarship

- Coauthored 50 peer-reviewed journal articles
- Cited over 1250 times with an h-index of 19 (19 articles with at least 19 citations), according to Google scholar.
- Current research in computational chemistry
 - Developing methods related to structure-based drug design
 - predicting binding affinities
 - simulating biological macromolecules
 - Involved in virtual screening projects for antibiotic drug discovery
 - research funded by NIH and NSF

Full curriculum vitae: http://mypages.iit.edu/~dminh/DavidMinh_CV.pdf

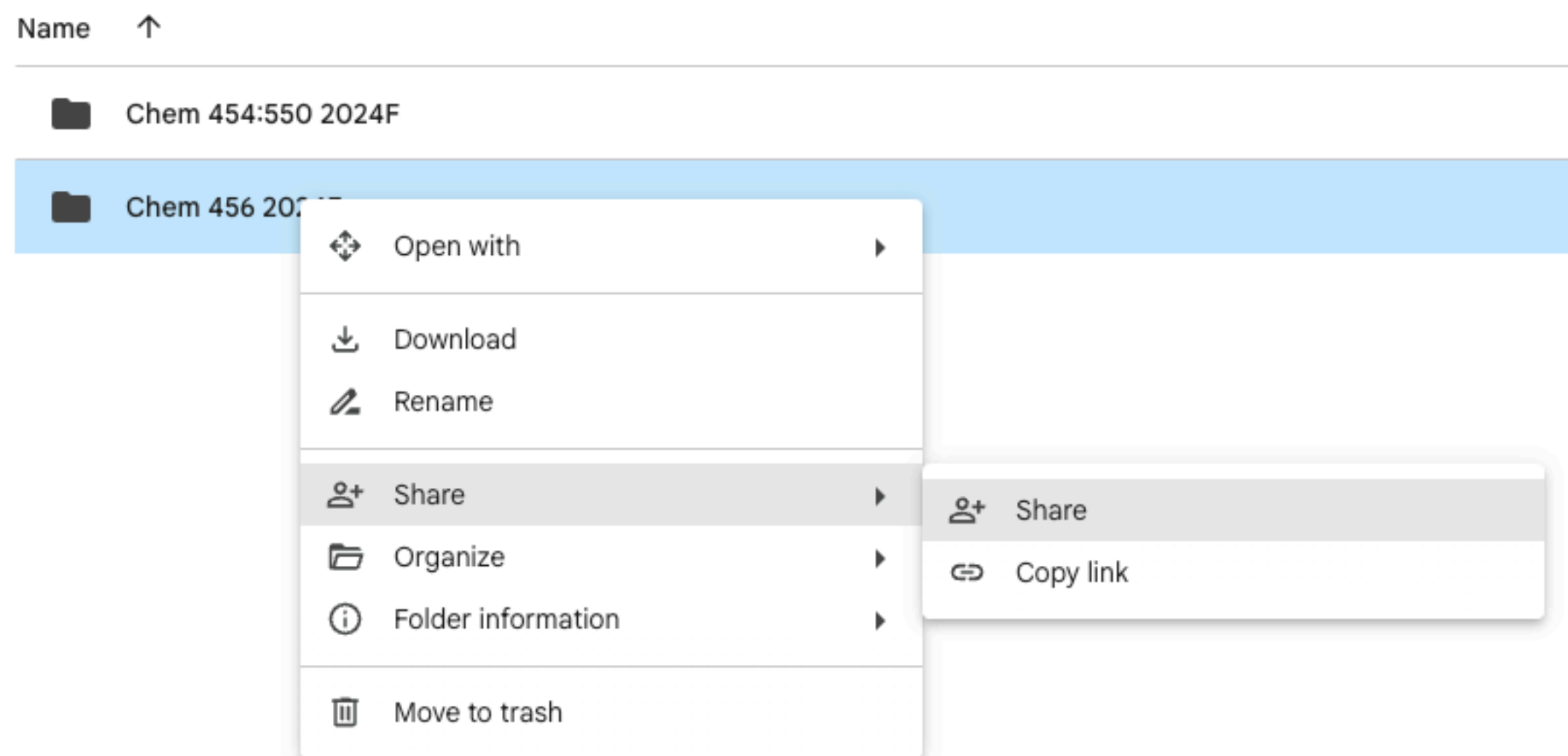
About me: beyond work

- Outside of work, I like to
 - play sports, especially Taekwondo, tennis, and basketball
 - play chess and other games, especially strategy and word games
 - read news and sometimes books
 - listen to podcasts and audiobooks. Some of my favorite podcasts are Hidden Brain and Planet Money.
 - travel. I've been to 6 continents
- I used to, but now not as often,
 - play music
 - play video games with my kids
- I am
 - Australian-born and American-raised by Vietnamese parents of Vietnamese and Chinese descent
 - married, with 2 children
 - Christian
 - incredibly blessed!

[Introduce yourself]

- What is your full name? What do you like to be called?
- Which degree program are you in?
- What are you hoping to learn in this class?
- How will this help you achieve your goals?
- Share something interesting about yourself

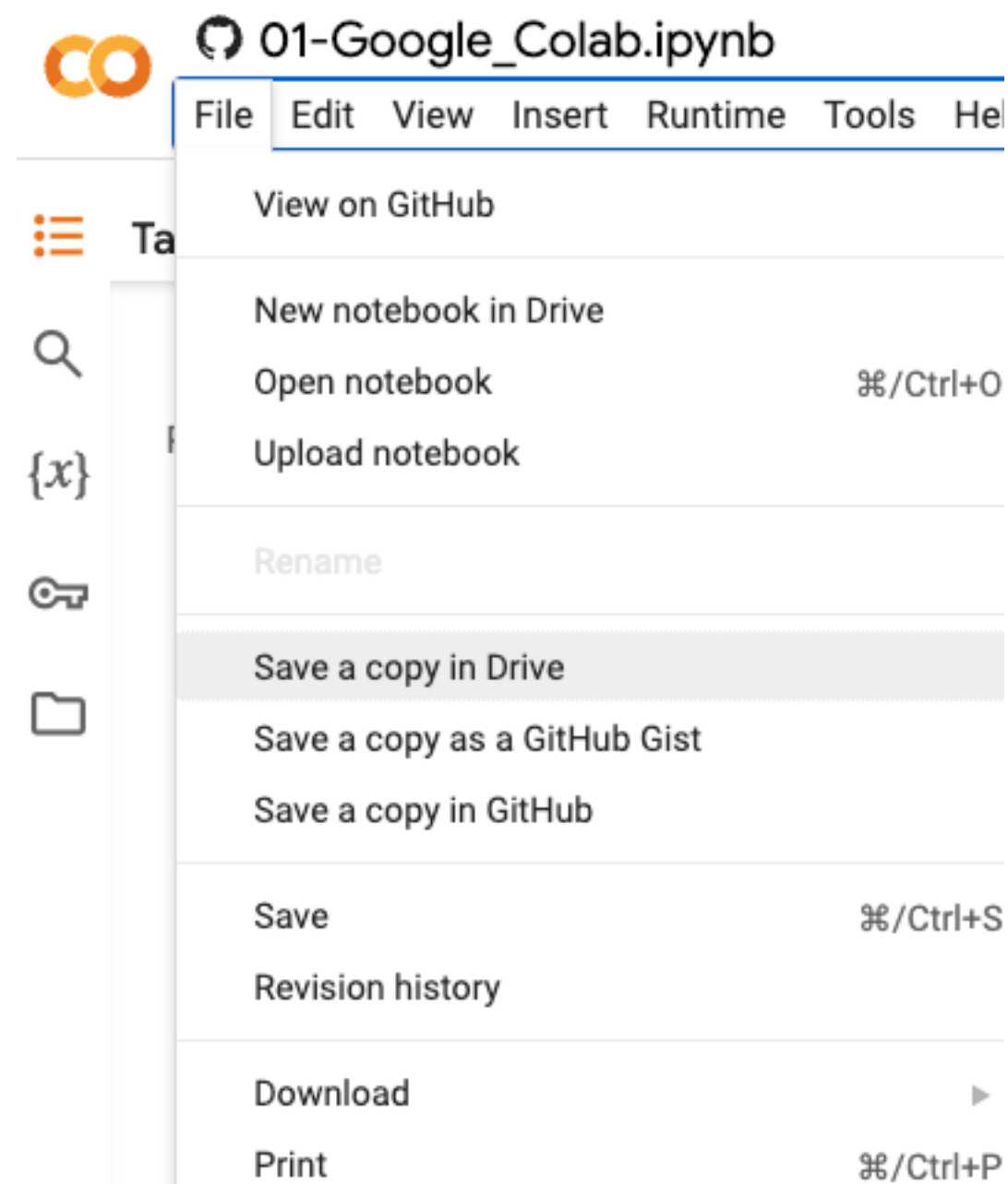
Google Drive Folder Setup



- Log in to Google Drive. This can be a school account or a personal account.
- Create a folder for this class called “Chem456-2024F”
- Create the subfolders “exercises” and “quizzes”
- Right click on the folder.
- Select “Share”
- Share the folder with me, dminh@iit.edu, and the TA, tnguyen48@hawk.iit.edu.

Exercise 1: Introduction to Google Colab

https://colab.research.google.com/github/daveminh/Chem456-2024F/blob/main/exercises/01-Google_Colab.ipynb



- After following this link, you should
 - save a copy of the notebook to Google Drive
 - rename it to 01-Google_Colab.ipynb
- move it to your class folder under the “exercises” folder
- work on and save the notebook