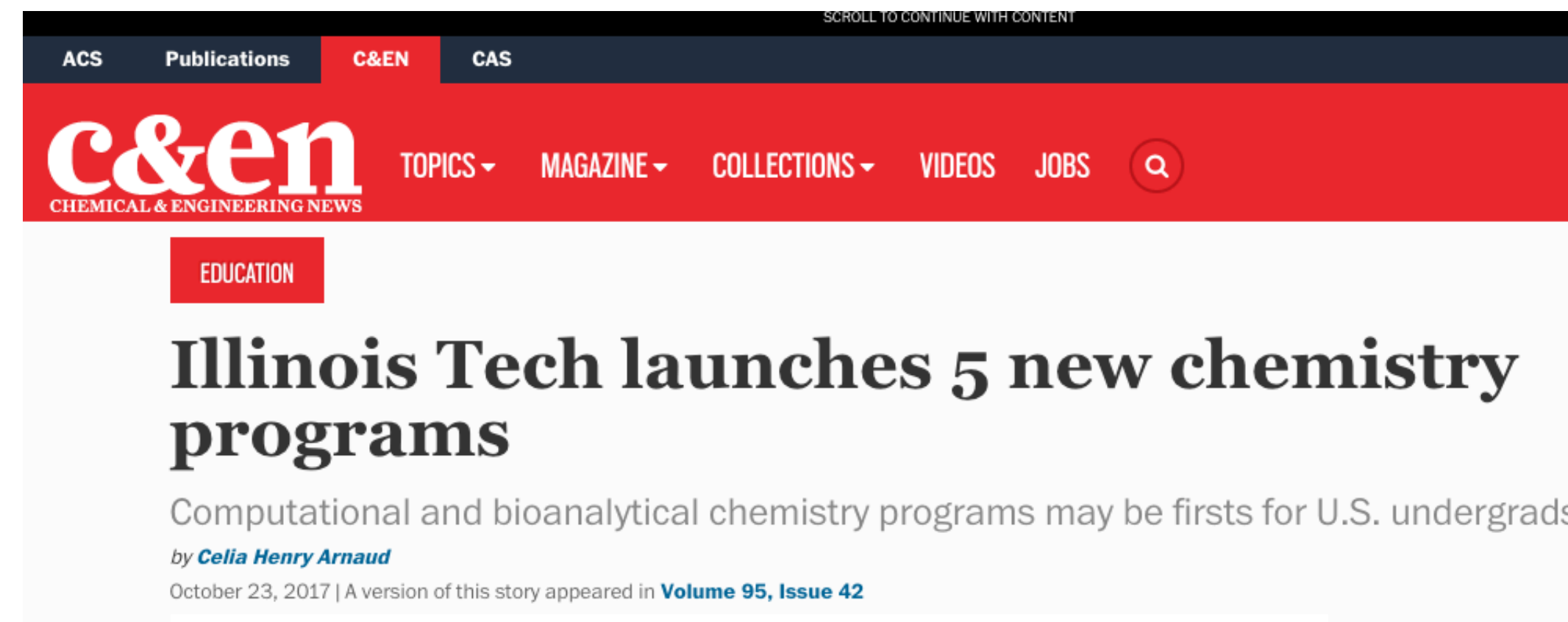


# 8/22/2022

- 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.

# Syllabus

<https://daveminh.github.io/Chem456-2022F/>

# Introductions

# About me: work

## Biographical

### Professional History

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

### Education

2004 – 2007	<b>Ph.D. in Physical Chemistry</b> , 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>B.A. in Chemistry</b> , 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](http://mypages.iit.edu/~dminh/DavidMinh_CV.pdf)

# About me: beyond work

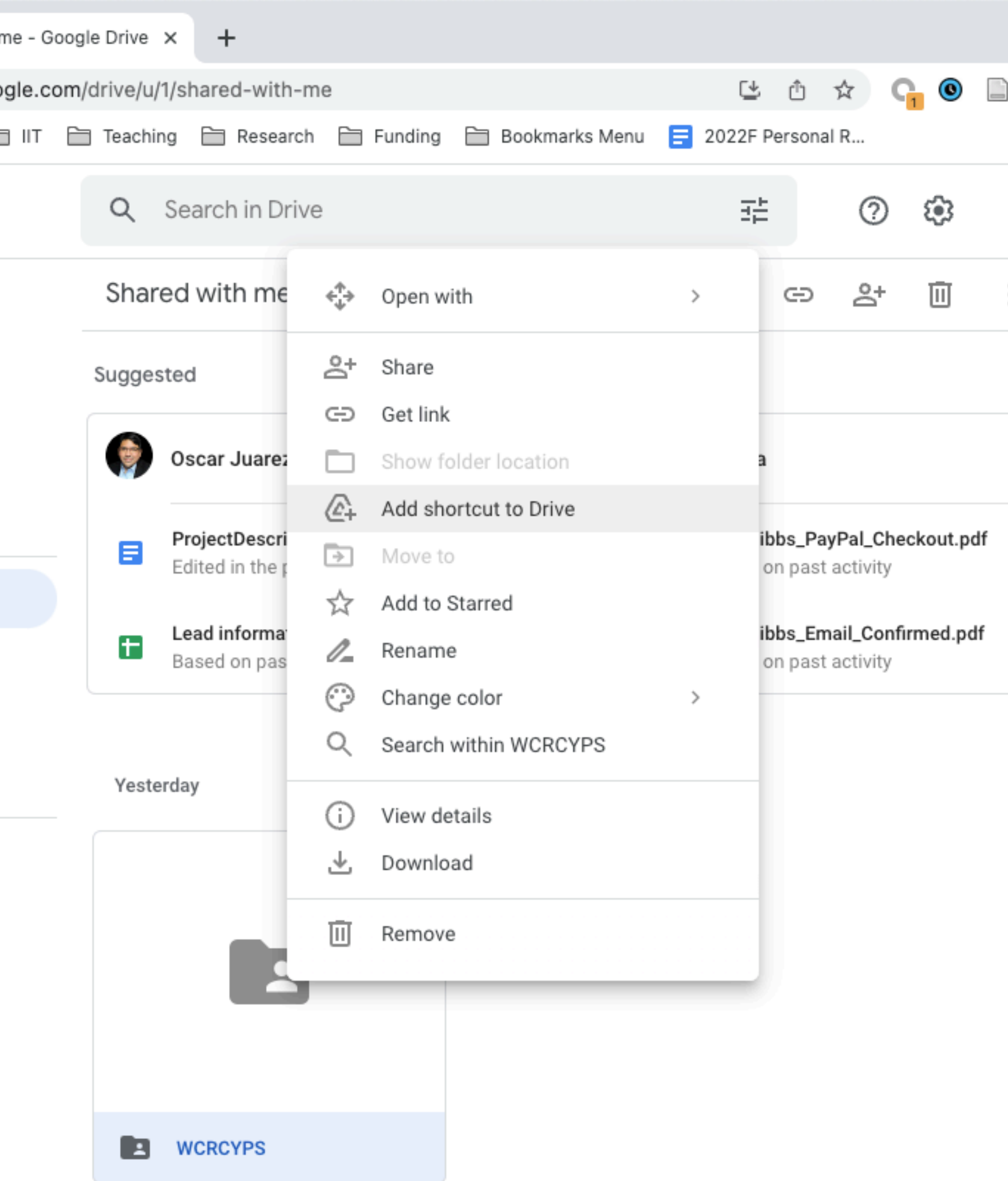
- Outside of work, I like to
  - play chess and other board games, especially strategy and word games.
  - play music, especially classical piano. Sometimes I also play guitar and bass.
  - listen to podcasts and audiobooks. Some of my favorite podcasts are Hidden Brain, Planet Money, and Invisibilia from NPR, and Revisionist History by Malcolm Gladwell.
  - read news and sometimes books
  - play video games with my kids, especially on Nintendo Switch
  - play sports, especially Taekwondo, tennis, and basketball. I also like hockey but haven't played in a while.
  - exercise, especially weights, swimming, biking, and skiing
  - travel. I've been to 6 continents
- I am
  - Australian-born and American-raised by Vietnamese parents of Vietnamese and Chinese descent
  - married, with 2 children
  - Christian
  - incredibly blessed!

# [Introduce yourself]

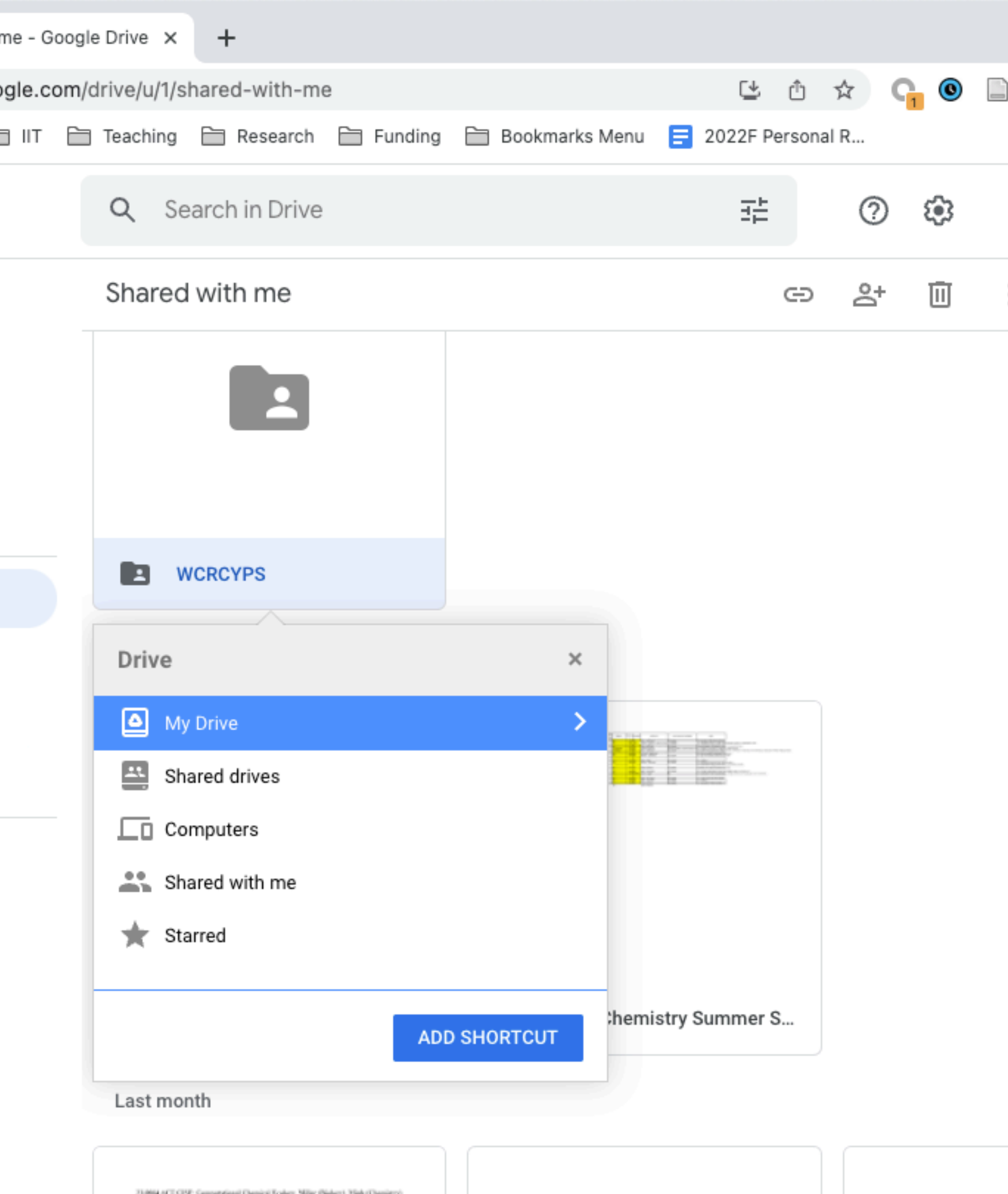
- What is your full name? What do you like to be called?
- Which degree program are you in?
- What are you hoping to learn in this class?
- How will this help you achieve your goals?
- Share something interesting about yourself

# **Google Drive Folder Link Setup**

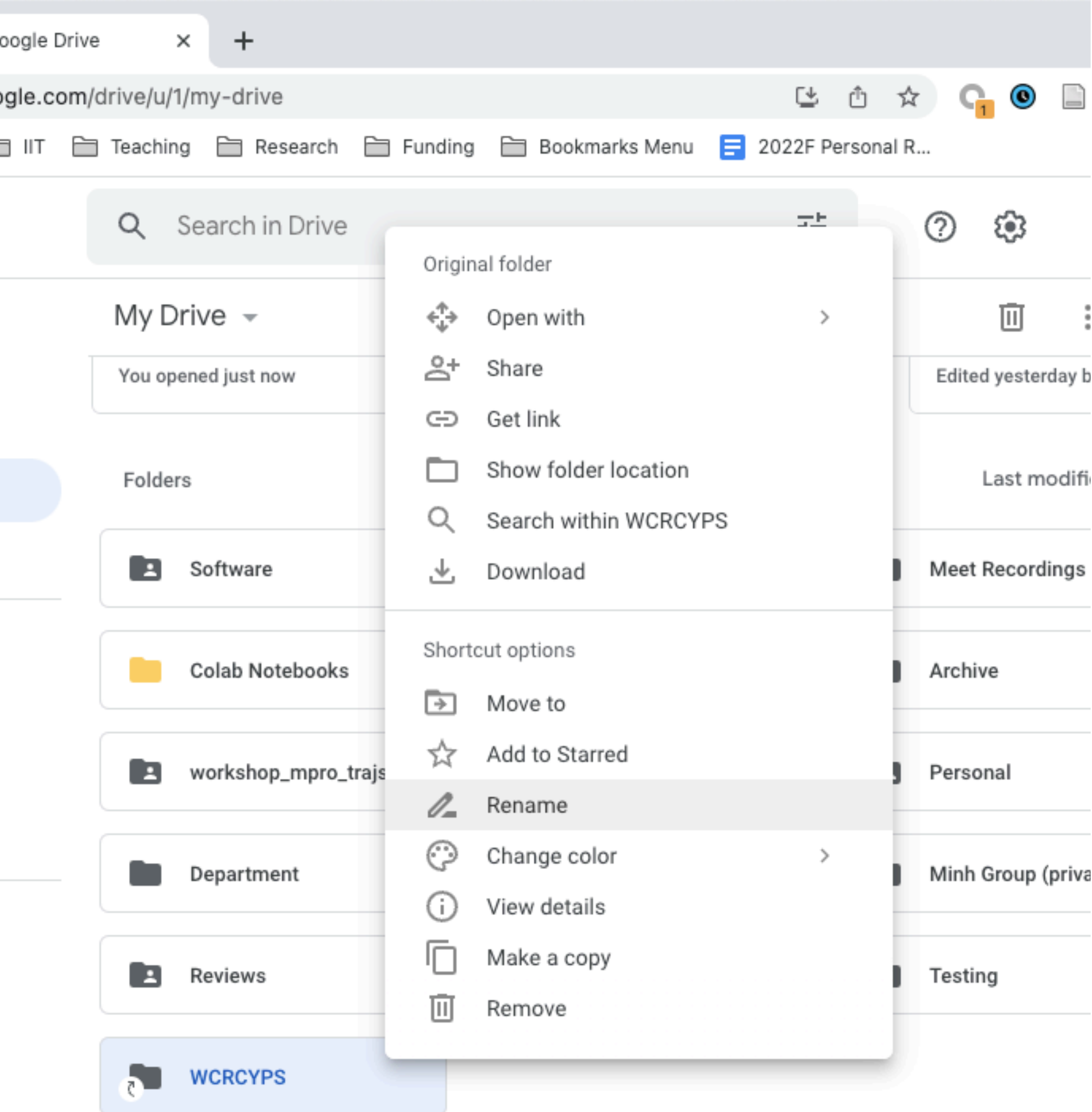




- Log in to Google Drive.
- Find the folder that I have shared with you under “Shared with me”.
- Here, I am creating a link to a folder called “WCRYCPS”, but you will link to a folder with your IIT user name that I shared with you.
- If I have not shared a link to the folder with you, then email me and ask me to do so.
- Right click on the folder.
- Select “Add shortcut to Drive”.



- Click on “My Drive” and then “Add Shortcut”
- There should be a small popup that says “Shortcut added to My Drive”



- Now navigate to “My Drive”
- Find the shortcut to the folder.
- Right click on the shortcut and select “Rename”
- Rename the shortcut to “Chem456-2022F”. This is where the labs expect your data to be. If you do not take this step, you will have to do more work to change the labs later in the semester.

# Exercise 1: Introduction to Google Colab

colab