CHEM 353e: Topics in Materials Science  
Fall 2017

General Information

Instructor:  Prof. Joshua Schrier  
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Office hours:  tba, and by appointment

Class:  Tuesday and Thursday from 10:00-11:30 a.m., KINSC Sharpless 416 (SHA416).  
(Second half of the Fall semester)

Prerequisites:  
(One junior-level Chemistry course)  
OR (one sophomore-level physics/computer science AND one 100-level Chemistry)

Text:  One required texts: 

Michael Nielsen, Reinventing Discovery: The New Era of Networked Science 
(Princeton Univ. Press, 2011) 272pp.  Please note that this is available as a free 
download via the Tri-Co Library

Online Texts:  Other articles will be posted on Moodle as required reading.  You will 
also make extensive use of online journals during the preparation of your proposal.

Topics:  This course will focus on data-driven collaborative approaches for chemistry/materials 
discovery and development, motivated in part by the United States’ Materials Genome 
Initiative and similar funding initiatives abroad.

To get started, we will take a look at some overviews of the Materials Genome 
Initiative, and the use of large-scale computation, databases, and machine learning in 
materials science.  We will then do a “deep dive” into case studies on some existing 
projects focusing on organic, inorganic, and biomaterials.  We will use the existing 
materials/chemistry projects as concrete examples to think about how to apply these 
strategies can be applied to materials/chemical problems, and to reflect upon the 
successes and shortcomings of existing projects.  In parallel, we’ll read and discuss a 
book on collaborative ways to do “open science”.  We’ll also discuss strategies for 
database design.

Your goal for the class is to develop a proposal for a new data-
driven/collaborative/online project to assist in chemical/materials discovery.  You 
are strongly encouraged to choose an area related to your current (or future) research 
interests.  The ideal outcome is an exciting (competitive/fundable) proposal that would 
dramatically improve chemical/materials research efforts, that you could use for future 
senior thesis research, business plans, graduate fellowships applications, etc.

Grades:  Grades will be calculated on the following basis:  (see below) 

  20% In-class participation/discussion  
  20% Out-of-class participation via Forum & File Uploads  
  10% Lightning talk (1 minute presentation)  
  15% Written Pre-proposal (1-2 page)  
  15% Final Oral presentation (10-15 minutes)  
  20% Final Written Proposal (<15 pages)

Attendance:  Attendance at all class sessions is a requirement of this course.  This is not a lecture 
course; you will be expected to discuss the material in a seminar-type setting.  Any 
planned absence (i.e., for athletic events or other special circumstances) must be 
discussed with the instructor as soon as possible.
Pre-class Readings: Readings from the text will be assigned before each class; it is paramount that you do this reading before each class. Expect to read about 50 pages before each class. Class time will be based on the assumption that you have done the reading—Don’t show up “unarmed” to a battle of wits!

Getting Feedback/Out of Class Participation:
Since this course explores non-traditional ways of doing science, it seems quaint to stick solely to the traditional forms of assessment (papers, presentations, etc.). To improve the extent and immediacy of feedback that you can get from your peers (and from me), I want us to make extensive use of the Moodle Forum.

I hope that you will share interesting articles that you come across in the literature, continue the discussion “out of class” by finding and sharing relevant articles and ideas, and as a place for public brainstorming and critique of your pre-proposals and proposals. To incentivize this, deliverable (“goal”) is 1 meaningful “new” post and 5 meaningful comments on other posts. But I hope that you will find this intellectually fun/challenging/interesting and will exceed this minimum quota.

Case-Studies: We discussing some existing projects so that we have concrete examples. Before each case study discussion in class, I would like each of you to identify at least one relevant paper (that was not part of the assigned reading), upload it to Moodle, and be prepared to discuss it in connection to the reading.

Note that this class will involve lots of new terminology and jargon and a wide range of scientific fields. Be sure you understand the science problem—the gold standard here is reading review articles that help “explain” the state of the field, but often a quick glance at Wikipedia can help give you the necessary initial context. Knowing when to skim and when to dive in is an important skill. When in doubt, read!

Topics for Case Studies:

- Organic materials for electronics and solar cells (Aspuru-Guzik & co.)
  - From material design to the Clean Energy Project
    - http://cleanenergy.molecularspace.org/
- Metal organic frameworks and zeolites for gas storage and separation (Snurr/Haranczyk/Smit & co.)
  - http://hmofs.northwestern.edu
  - https://mof1.cchem.berkeley.edu/ccmdb/index.php
- Data-driven protein design (Baker & co.)
  - Interplay of Monte Carlo optimization, bonding models, and automated experiments
- Organic reaction planning (e.g., Grzybowski, Jensen, Waller, etc.)
  - From DENDRAL to Chematica and beyond
  - Dial-a-molecule http://generic.wordpress.soton.ac.uk/dial-a-molecule/
- Computational solid-state thermodynamics and phase diagrams (e.g., Wolverton, Ceder, Persson)
  - Computational screening of inorganic materials for Li-ion batteries
    - https://materialsproject.org
  - “Phase diagram of the earth”
    - http://wolverton.northwestern.edu/news/oqmdwebsiteislive
Lightning Talks: You’ll have a chance to “pitch” your project to the class, in the form of a one-slide, one-minute talk. We’ll then offer feedback. Lighting talks will be held at the beginning of class on Tuesday, 21 Nov 2017; please upload your slides to the Moodle Directory before class.

Pre-proposal: By the time we get half-way through the course, you will have seen several examples of large databases for materials discovery, and explored some of the patterns (and challenges) in developing these types of resources. At this stage you should have an idea of what chemical/materials problem you want to tackle and some ideas on how to do this. I am also happy to brainstorm with you throughout the class (and during office hours) on possible projects. Since this course is nominally a materials science course, I would prefer if you chose a materials related problem. However, any chemical problem with some functional/application aspect is acceptable.

In your 1-2 page pre-proposal you will provide a summary of your proposed research project. Succinctly state the fundamental scientific problem to be addressed, outline the significance of the problem, the originality of the approach, and the impact it may have on the field if it is successful. You do not need an extensive bibliography, but plan to cite 2-3 relevant papers. The purpose of this is to clarify your idea and also to get formal feedback.

Pre-proposals are due Thursday, 30 Nov 2017. Upload your pre-proposals (in Microsoft word .docx format) to the relevant folder on Moodle.

Presentations: The final week of class (12-14 Dec) will be spent on short presentations, where you will “pitch” your project to the class. Depending on enrollment, these will be 15-30 minute long; you are encouraged to use PowerPoint-type presentation software to enhance the effectiveness of your presentation by using graphics where appropriate. The purpose of this is twofold: (i) to gain experience in public oral presentations; (ii) to get more detailed feedback from your classmates and I on your project.

Upload a PDF of your slides to the relevant folder on Moodle before your presentation.

Final Proposal: Your final deliverable is to a ≤15 page proposal that lays out the intellectual merit for your project and describes the initial steps you would take to turn your project into a reality. You should model this on the National Science Foundation proposal format (http://www.nsf.gov/pubs/2004/nsf04016/start.htm) except, you should not worry about writing about Broader Impacts, Education and Human Resources Goals, Biographical Sketches, Budgets, Current and Pending Support, or Facilities. In other words, I want you to solely focus on the proposal narrative. The final papers are due on Friday, 22 Dec at noon, to by upload to Moodle (in Microsoft Word .docx format). What should they look like?

Guidelines for an NSF-style Proposal:

There are many resources on the web for writing “successful” NSF proposals, e.g., http://www.cs.cmu.edu/~sfinger/advice/advice.html

Generally, they all recommend very similar compositions:

I’ll leave it up to you if you want to write a Project Summary page (+1 page). It is not necessary, but you might enjoy concluding your work in this way. It will also give you a chance to revise and refine your
The Narrative (≤15 pages) consists of:

1-2 pages putting your work into a broader context—what sorts of problems will this solve on the 10-20 year timeframe? Why is the problem you are solving relevant to society? Dedicate 1-2 paragraphs summarizing your current (proposed) contribution.

2-3 pages discussing the current/existing work in the field. What is already out there? How is what you are proposing different from that?

5-7 pages discussing what you plan to do. Preliminary results (if they exist) are good. For this project, you might want to include “mock ups” (i.e., pretty pictures that show what a user interface might look like) to help illustrate your proposal.

Generally this contains a mix of projects. In “real life”, about a third should be problems that you have mostly finished solving already (this helps you establish credibility); these are the ones you will tackle in the first year of your project. A third are problems that you have some clear ideas on how to solve, but haven’t done yet. And a third are long range projects, that you will tackle towards the end of your project. Since you’ll be learning lots of things, you don’t necessarily have to have a precise plan for how to solve these. However, for the purposes of this class: you probably haven’t solved any problems yet, so don’t worry about this.

Conclusion: A paragraph or two summarizing why your research is important, etc.

Use figures as appropriate. These do count against your 15 page limit.

References, as appropriate. Include these at the end, after your narrative is over. These do not count against your 15 page limit.

**Honor Code:** The Haverford College Honor Code, as outlined in the Haverford College Catalog and administered by the Honor Council, applies to all submitted work in CHEM 353g. Students are encouraged to collaborate, but it is a requirement that all submitted material be your own; this includes plots and graphics generated using a computer. You must acknowledge in writing (and properly cite) any assistance or material from the literature, other students, textbooks, internet, or any source but Prof. Schrier. Please consult Prof. Schrier if you have any questions regarding the Honor Code.

**Accommodations:** Haverford College is committed to supporting the learning process for all students. Please contact me as soon as possible if you are having difficulties in the course. There are also many resources on campus available to you as a student, including the Office of Academic Resources (https://www.haverford.edu/oar/) and the Office of Access and Disabilities Services (https://www.haverford.edu/ads/). If you think you may need accommodations because of a disability, please contact Sherrie Borowsky, Coordinator of Accommodations, Office of Access and Disability Services at hc-ads@haverford.edu. If you have already been approved to receive academic accommodations and would like to request accommodations in this course because of a disability, please meet with me privately at the beginning of the semester (within the first two weeks if possible) with your verification letter.

**For more info:** Consult the course Moodle site at https://moodle.haverford.edu/course/view.php?id=475