MSE 598 – Solid State Ionics
Fall 2020

Instructor: Prof. Nicola H. Perry
Nominal Class Time: Tu & Th 9:30-10:50 AM

Note: For the online version of this course, the nominal 160 minutes of in-class time per week will be split between synchronous discussions (on Zoom) and asynchronous pre-recorded lectures (on Compass). I will endeavor to not go over the allocated total time so that the online version does not end up being more work than an in-person class. This means that our Zoom discussions will not typically take up the full 9:30-10:50 AM slot. Discussions on Zoom will include: answering your questions about lecture content, summarizing the important points, presenting case studies and real-world examples of the material from lectures (e.g., news/research highlights), and student presentations. The purpose of discussions is like office hours: to help you understand and apply the lecture material and connect it to relevant applications.

Email:	nhperry@illinois.edu (write "MSE 598" in the subject line) – *Piazza is preferred*
Discussion:	*Zoom*, Tu & Th 9:30AM-
Office Hours:	*Zoom*, During discussion sessions (also available by appointment)
Course Website:	*Compass* (https://compass2g.illinois.edu/webapps/login/)
Lectures:	Posted on *Compass* (asynchronous – watch when it's convenient for you)
Quiz Study Guides:	Posted on *Compass*
Readings:	Posted on *Compass*
Presentation Guide:	Posted on *Compass*
Discussion Board:	*Piazza* – share questions, links, documents with the class & instructor
Assignments:	Turn in on *Gradescope*
Quizzes:	On *Gradescope*

Primary Text:
1. *Physical Chemistry of Ionic Materials: Ions and Electrons in Solids* by Joachim Maier – free e-book available through the library

Supplemental Texts:
1. *Defects in Solids* by Richard Tilley – free e-book available through the library
2. *The Defect Chemistry of Metal Oxides* by D.M. Smyth, Oxford University Press: New York (2000) – at Grainger Engineering Library
3. *Solid State Electrochemistry I* and *Solid State Electrochemistry II* edited by V.V. Kharton – free e-books available through the library
4. *Solid State Electrochemistry* by Peter Bruce – free e-book available through the library
5. *Defects and Transport in Crystalline Solids* by Per Kofstad and Truls Norby – free e-book available online through on-campus internet or VPN
6. Additional readings from recent literature – will be listed on Compass and accessible online through the on-campus internet or VPN

Prerequisites:
Some familiarity with thermodynamics and ionic materials (e.g., oxides) through research or coursework will be helpful (e.g., MSE 403, 420, or 422)

Class Description and Objectives:

General Objective:
My goal as the instructor is to serve students through clear teaching and accessible and engaging discussions so that you can explore, understand, apply, and hopefully enjoy Solid State Ionics.

Specific Objectives:
Students will be able to:
1) calculate point defect concentrations using formation energies, develop Brouwer diagrams, describe several means of tailoring point defect concentrations through independent variables, and apply equilibrium thermodynamics to the case of defective solids
2) write point defect reactions in Kroger-Vink notation to describe defect processes, and apply a non-equilibrium thermodynamics and chemical kinetics framework to describe defect reactions and kinetic behavior
3) describe operation of various solid state ionics applications (including open circuit cells, cells using current, and cells generating current)
4) select measurement techniques appropriate for investigating solid state electrochemical material/device behavior and select materials appropriate for different functions within the devices
5) use appropriate resources for finding up-to-date information on solid state ionics for continued learning

Course readings, videos, discussions, quizzes, and assignments are designed to help students make progress toward these objectives. Assessment (grading) will be based on demonstrated student learning gains towards these objectives.

Course catalog description of content:
Solid state ionic materials applied in energy conversion, energy storage, catalysis, sensing, responsive coatings, neuromorphic computing, and memory. Underlying point defect behavior, i.e., transport and reactions, through equilibrium thermodynamics, chemical kinetics, and irreversible thermodynamics. Practical solid state electrochemistry techniques and case studies.

Class Outline & Topics:

Note: Instructor reserves option to remove or add topics as necessitated by time constraints

Introduction to Solid State Ionics (e.g., Tuller & Knauth 2004 article)
- Applications
- Underlying defect processes
- Recent developments & open questions

Review (e.g., Kofstad & Norby pp. 1-21)
- Bonding in ceramics
- Crystal structures
- Processing

Equilibrium Thermodynamics Applied to Defective Solids (e.g., Maier Chapter 5)
- Point defect formation (electronic, ionic)
- Defect reactions, association, internal/external defect equilibria, doping
- Brouwer diagrams
- Higher-dimensional defects
- Interfacial defect chemistry and size effects
- Chemo-mechanical coupling
- Photo-ionics

Chemical Kinetics & Irreversible Thermodynamics (e.g., Maier Chapter 6)
- Transport & reactions
- Mobility – ionic/electronic, isolated vs. concerted hopping, mechanisms of charge migration
- Various diffusion constants: self-diffusion, tracer diffusion, chemical diffusion
- Surface reactions & catalysis

- Solid state reactions
- Concentration profiles
- Non-linear phenomena far from equilibrium (time permitting)

Measurement Techniques & Ionics Applications – Solid State Electrochemistry (e.g., Maier Chapter 7)
- Open circuit cells, cells under current, cells generating current
- Techniques: cell and electrode design, impedance spectroscopy, coulometric titration, stoichiometry polarization, pumping cells, thermogravimetric analysis, various relaxation approaches, optical methods, etc.
- Batteries
- Membranes & filters
- Fuel & electrolysis cells
- Solar thermo-chemical reactors
- Sensors
- Electrochemical pumps
- Memristors & neuromorphic computing

In-Depth Case Studies (e.g., Kharton select chapters)
- Materials for electrolytes & superionic conductors
- Materials for electrodes

Grading Policies:
Learning gains will be promoted and assessed with the following assignments:
- Homework (15% of total grade)
  - There will be approximately 4±1 assignments throughout the semester.
  - Assignments will be turned in on Gradescope.
- Presentations (15% of total grade)
  - Students will present short ~5-10 minute summaries and analysis of recent key journal articles in the field of solid state ionics, using Powerpoint (or equivalent) slides.
  - Papers should be shared with the class at least a day in advance of the presentation.
  - Each student will present twice throughout the semester, to enable feedback and improvement.
- Quizzes (35% of total grade)
  - There will be quizzes approximately every 2 weeks throughout the semester.
  - Quizzes will cover materials presented in class, in readings, and on homework.
- Written Lecture Question Summaries (15% of total grade)
  - Due each week prior to relevant Zoom discussions
  - Write 3 questions that came up as you watched the videos and answer 1 of them
  - Graded on clarity, precision, completeness
  - Indicate with asterisk (*) questions you would like to be discussed in Zoom discussion
- Participation (5% of total grade)
  - Classes such as this are greatly improved by active discussion and participation.
  - You could participate by, for example: 1) asking questions after student presentations, 2) asking questions during discussions, 3) answering students' questions on Piazza, 4) participating in discussions, 5) sharing research articles/ news during discussions that's relevant to the lecture content, etc.
  - Attendance at Zoom discussions will count toward your participation grade
- Term paper (15% of total grade)
  - Students will write a proposal-style report describing a potential new opportunity for development/understanding of solid state ionics materials, measurement or simulation approaches, or applications. This must be different than students' existing research.
  - Papers will be turned in electronically, and portions of the written assignments will be due at different times through the semester, to enable feedback.

Late Homework Assignments:

- 20% of total available score lost per day late (unless for a valid, documented reason)
- If you have a valid, documented reason for a late assignment, I can discuss this on a case-by-case basis

Late Quizzes/ Papers/ Lecture Question Summaries:

- <u>No credit for late submission</u>
    - Reasons: fairness of the quiz process; paper due date is at end of course and I need enough time to grade; lecture questions are used in Zoom discussions
- If you anticipate needing to re-schedule a quiz for a documented, valid reason, please let me know as far in advance as possible because these are programmed in the online system to be available at a certain time.
- I recommend having a back-up internet access method (e.g., wi-fi vs. phone/ multiple wi-fi options) to ensure that connectivity issues don't prevent you from completing a quiz/ meeting a due date.
- Documented, valid emergencies causing you to miss a deadline for one of these can be discussed on a case-by-case basis.

Academic Code of Conduct:

- Students are referred to the University of Illinois, Urbana-Champaign Student Code for complete details on expectations for academic integrity (http://studentcode.illinois.edu/). Special attention should be given to Part 4 of Article 1.
- Cheating and plagiarism will be addressed according to established campus policy. Students found cheating or plagiarizing will receive a failing grade.

Disability Accommodations:
To determine if you qualify for disability-related academic adjustments and/or auxiliary aids, students with disabilities must contact the course instructor and the Disability Resources and Educational Services (DRES) as soon as possible. To contract DRES, you may visit 1207 S. Oak St., Champaign, call 333-4603 (V/TTY), or email a message to disability@uiuc.edu.

Diversity:
I greatly value the diversity that students bring to the (virtual) classroom, particularly in a discussion/presentation-heavy class such as MSE 598. I learn a lot from your questions, ideas, interests, and comments. Together as a class, our perspective on the science and applications is greatly broadened when everyone participates. More generally, it's clear that diverse participation in engineering is needed to ensure that technology is designed to serve and be accessible to the whole population rather than a narrow subset. In science, diverse perspectives and lenses benefit the whole community through increasing creativity and innovation. Further, in the context of increasing globalization, students need to be well prepared for teamwork and communication in a diverse and international setting to address challenges where Solid State Ionics knowledge can assist (e.g., climate change, disease epidemics, water accessibility, sustainable energy, etc.). My goal is to create an inclusive classroom environment where all students can take risks to fully participate and thereby grow and learn. If you have suggestions for the instructor on improving the course environment and culture from a diversity perspective, please do reach out.