MSE 598 – Solid State Ionics
Fall 2021

Instructor: Prof. Nicola H. Perry
Class Time: Tu & Th 9:30-10:50 AM
Class Location: CIF (Campus Instructional Facility) room 2036

Email:	nhperry@illinois.edu ("MSE 598" as subject line); *Canvas discussion preferred*
Office Hours:	*Zoom*, times TBD depending on students' input; *Zoom* link posted on *Canvas*
Course Website:	*Canvas* (https://canvas.illinois.edu/courses/13836)
Discussion Board:	*Canvas*
Assignments:	Posted and turned in 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:
- Quizzes (45% 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.
- Homework (20% of total grade)
  - There will be approximately 4±1 assignments throughout the semester.
- 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.
- Presentations (10% of total grade)
  - Students will present short 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 a week in advance of the presentation.
- Participation (10% 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 or answering questions during class, 3) summarizing small-group discussions in class, 4) sharing research articles/ news during class that are relevant to the content, etc.

Late Homework Assignment Policy:
- *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/ Presentations Policy:
- *Lowest quiz grade automatically dropped*
- No credit for late submission
  - Reasons: fairness of the quiz process; I need enough time to grade
- If you anticipate needing to re-schedule a quiz for a documented, valid reason, please let me know as far in advance as possible.
- 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 Integrity:
The University of Illinois at Urbana-Champaign Student Code should also be considered as a part of this syllabus. Students should pay particular attention to Article 1, Part 4: Academic Integrity. Read the Code at the following URL: http://studentcode.illinois.edu/.
Academic dishonesty *may result in a failing grade*.

Every student is expected to review and abide by the Academic Integrity Policy: https://studentcode.illinois.edu/article1/part4/1-401/. Ignorance is not an excuse for any academic dishonesty. It is your responsibility to read this policy to avoid any misunderstanding. *Do not hesitate to ask the instructor* if you are ever in doubt about what constitutes plagiarism, cheating, or any other breach of academic integrity.

Disability-Related Accommodations:
To obtain 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 contact DRES, you may visit 1207 S. Oak St., Champaign, call 333-4603, e-mail disability@illinois.edu or go to https://www.disability.illinois.edu. If you are concerned you have a disability-related condition that is impacting your academic progress, there are academic screening appointments available that can help diagnosis a previously undiagnosed disability. You may access these by visiting the DRES website and selecting "Request an Academic Screening" at the bottom of the page.

COVID-Related Policies:
Following University policy, all students are required to engage in appropriate behavior to protect the health and safety of the community. Students are also required to follow the campus COVID-19 protocols.
Students who feel ill must not come to class. In addition, students who test positive for COVID-19 or have had an exposure that requires testing and/or quarantine must not attend class. The University will provide information to the instructor, in a manner that complies with privacy laws, about students in these latter categories. These students are judged to have excused absences for the class period and should contact the instructor via email about making up the work.
Students who fail to abide by these rules will first be asked to comply; if they refuse, they will be required to leave the classroom immediately. If a student is asked to leave the classroom, the non-compliant student will be judged to have an unexcused absence and reported to the Office for Student Conflict Resolution for disciplinary action. Accumulation of non-compliance complaints against a student may result in dismissal from the University.

All students, faculty, staff, and visitors are required to wear face coverings in classrooms and university spaces. This is in accordance with CDC guidance and University policy and expected in this class.
Please refer to the University of Illinois Urbana-Champaign's COVID-19 website for further information on face coverings. Thank you for respecting all of our well-being so we can learn and interact together productively.

In order to implement COVID-19-related guidelines and policies affecting university operations, instructional faculty members may ask students in the classroom to show their Building Access Status in the Safer Illinois app or the Boarding Pass. Staff members may ask students in university offices to show their Building Access Status in the Safer Illinois app or the Boarding Pass. If the Building Access Status says "Granted," that means the individual is compliant with the university's COVID-19 policies—either with a university-approved COVID-19 vaccine or with the on-campus COVID-19 testing program for unvaccinated students. Students are required to show only the Building Access Screen, which shows compliance without specifying whether it was through COVID-19 vaccination or regular on-campus testing. To protect personal health information, this screen does not say if a person is vaccinated or not. Students are not required to show anyone the screen that displays their vaccination status. No university official, including faculty members, may ask students why they are not vaccinated or any other questions seeking personal health information.

Diversity:
I greatly value the diversity that students bring to the 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.

Inclusivity Statement from the College:
The Grainger College of Engineering is committed to the creation of an anti-racist, inclusive community that welcomes diversity along a number of dimensions, including, but not limited to, race, ethnicity and national origins, gender and gender identity, sexuality, disability status, class, age, or religious beliefs. The College recognizes that we are learning together in the midst of the Black Lives Matter movement, that Black, Hispanic, and Indigenous voices and contributions have largely either been excluded from, or not recognized in, science and engineering, and that both overt racism and micro-aggressions threaten the well-being of our students and our university community. The effectiveness of this course is dependent upon each of us to create a safe and encouraging learning environment that allows for the open exchange of ideas while also ensuring equitable opportunities and respect for all of us. Everyone is expected to help establish and maintain an environment where students, staff, and faculty can contribute without fear of personal ridicule, or intolerant or offensive language. If you witness or experience racism, discrimination, micro-aggressions, or other offensive behavior, you are encouraged to bring this to the attention of the course director if you feel comfortable. You can also report these behaviors to the Bias Assessment and Response Team (BART) (https://bart.illinois.edu/). Based on your report, BART members will follow up and reach out to students to make sure they have the support they need to be healthy and safe. If the reported behavior also violates university policy, staff in the Office for Student Conflict Resolution may respond as well and will take appropriate action.

Sexual Misconduct Reporting Obligation:
The University of Illinois is committed to combating sexual misconduct. Faculty and staff members are required to report any instances of sexual misconduct to the University's Title IX Office. In turn, an individual with the Title IX Office will provide information about rights and options, including accommodations, support services, the campus disciplinary process, and law enforcement options.
A list of the designated University employees who, as counselors, confidential advisors, and medical professionals, do not have this reporting responsibility and can maintain confidentiality, can be found here: wecare.illinois.edu/resources/students/#confidential.
Other information about resources and reporting is available here: wecare.illinois.edu.

Religious Observances:
Illinois law requires the University to reasonably accommodate its students' religious beliefs, observances, and practices in regard to admissions, class attendance, and the scheduling of examinations and work requirements. You should examine this syllabus at the beginning of the semester for potential conflicts between course deadlines and any of your religious observances. If a conflict exists, you should notify your instructor of the conflict and follow the procedure at https://odos.illinois.edu/community-of-care/resources/students/religious-observances/ to request appropriate accommodations. This should be done in the first two weeks of classes.

Family Educational Rights and Privacy Act (FERPA):
Any student who has suppressed their directory information pursuant to Family Educational Rights and Privacy Act (FERPA) should self-identify to the instructor to ensure protection of the privacy of their attendance in this course. See https://registrar.illinois.edu/academic-records/ferpa/ for more information on FERPA.

Message from Campus Police:

Run > Hide > Fight

Emergencies can happen anywhere and at any time. It is important that we take a minute to prepare for a situation in which our safety or even our lives could depend on our ability to react quickly. When we're faced with almost any kind of emergency – like severe weather or if someone is trying to hurt you – we have three options: Run, hide or fight.

Run

Leaving the area quickly is the best option if it is safe to do so.

- Take time now to learn the different ways to leave your building.
- Leave personal items behind.
- Assist those who need help, but consider whether doing so puts yourself at risk.
- Alert authorities of the emergency when it is safe to do so.

Hide

When you can't or don't want to run, take shelter indoors.

- Take time now to learn different ways to seek shelter in your building.
- If severe weather is imminent, go to the nearest indoor storm refuge area.
- If someone is trying to hurt you and you can't evacuate, get to a place where you can't be seen, lock or barricade your area if possible, silence your phone, don't make any noise and don't come out until you receive an Illini-Alert indicating it is safe to do so.

Fight

As a last resort, you may need to fight to increase your chances of survival.

- Think about what kind of common items are in your area which you can use to defend yourself.
- Team up with others to fight if the situation allows.
- Mentally prepare yourself – you may be in a fight for your life.

Please be aware of people with disabilities who may need additional assistance in emergency situations.

Other resources

- **police.illinois.edu/safe** for more information on how to prepare for emergencies, including how to run, hide or fight and building floor plans that can show you safe areas.
- **emergency.illinois.edu** to sign up for Illini-Alert text messages.
- **Follow the University of Illinois Police Department** on Twitter and Facebook to get regular updates about campus safety.