CHEM 599
Molecular Electronics

Units: 2
Term—Day—Time: Spring 2025—MTh—15:30-17:10

Location: OCW 214

Start date: February 24, 2025
End date: May 02, 2025
(8 instructional weeks)

Instructor: Prof. Michael Inkpen
Office: LJS 250
Office Hours: by appointment.
Contact Info: inkpen@usc.edu, +1 (213) 821-1910.
Please allow 2 working days for a response to emails/calls.

Teaching Assistants: N/A
Office Hours: TBA

IT Help: N/A, use Blackboard.

Catalogue Description: Fundamental physical concepts, chemical principles, and potential applications of electronic components formed from single, or small groups of, molecules. Methods to form and study nanoscale molecular junctions, charge transport theory, structure-electronic property relationships. Operational characteristics of molecular wires, switches, diodes, and thermoelectric devices.

Course Description

CHEM 599: Molecular Electronics is a graduate level course covering the fundamental physical concepts, chemical principles, and potential applications of molecular-scale electronic materials. The intent of this course is to explain how single, or small groups of, molecules can function as electronic components such as wires, switches, or diodes. The properties of electrode-molecule-electrode junctions will be rationalized using ideas and tools spanning physical organic and inorganic chemistry, supramolecular chemistry, computational chemistry, and quantum mechanics. Topics may include charge transport theory, methods to form and manipulate molecular junctions, molecular structure-electronic property relationships, thermoelectricity, transport in biological systems, curation and development of the "Molecular Junction Database" for use as a literature search tool.

Learning Objectives

By the end of this course you should be able to:

- Contrast methods used to "wire up" and study individual and small groups of molecules into junctions.
- Evaluate and compare the conducting properties of different molecular compounds.
- Create new molecular junction database entries by reading, understanding, and extracting data from, recently published primary literature.
- Discuss the motivation(s) to study, and grand challenges to the implementation of, molecules as electronic circuit components.

By demonstrating that you can:

- Recognize and discuss key junction structure-electronic property relationships, rationalizing them using chemical principles.
- Interpret and assess experimental transport data using common theoretical models.
- Identify the electronic features characteristic of wires, switches, diodes, etc.
- Utilize simple computational experiments to provide insights into a molecule's electronic structure.
- Implement cheminformatics principles to convert figures and prose into machine-readable spreadsheet entries.

(These learning objectives are not comprehensive and subject to change.)

Prerequisite(s): N/A
Co-Requisite(s): N/A
Concurrent Enrollment: N/A
Recommended Preparation: N/A

COVID-19 Statement

If you test positive for COVID-19 during the semester, or experience any symptoms, you must not attend class in person until you obtain a negative test for COVID-19 and/or satisfy any recommended self-isolation requirements. If the lecture instructor tests positive for COVID-19 or experiences symptoms, lectures will be recorded on Zoom until they can safely return to teach in person.

Students are expected to comply with all aspects of USC's COVID-19 policy. Failure to do so may result in removal from the class and referral to Student Judicial Affairs and Community Standards. For latest information, see https://coronavirus.usc.edu.

Course Notes

Letter Grades will be assigned based on the assigments described below. Copies of lecture slides will be emailed to all registered participants. Poll Everywhere will be used, for example, to test understanding of key class concepts. Note that Poll Everywhere questions are not graded on right or wrong answers, only participation.

Technological Proficiency and Hardware/Software Required

Q-Chem – no prior experience required. Students can reserve time on a dedicated computer system to run their homework experiments remotely. Alternatively they can run these experiments on their own computer. A free USC site licence for Q-Chem is available, with install and operating instructions provided in class.

Required Readings and Supplementary Materials

Required Texts: None.

Supplemental Materials: Relevant literature readings will be assigned during the semester to reinforce/illustrate class discussions. Supplemental materials may be provided from various sources, including the following textbook(s) and review article(s):

(1) *Molecular Electronics: An Introduction to Theory and Experiment* (2nd Edition), Juan C. Cuevas and Elke Scheer; World Scientific Publishing Co. Pte. Ltd., ISBN-13: 978-9811225703

(2) *Chemical Principles of Single-Molecule Electronics*, T. A. Su, M. Neupane, M. L. Steigerwald, L. Venkataraman and C. Nuckolls, *Nature Reviews Materials*, **1**, 16002, 2016

Description and Assessment of Assignments

Poll Everywhere questions will be used periodically to encourage discussion and test understanding of key class concepts. Polls are graded only on participation, not on right or wrong answers.

Pop Quizzes will be periodically assigned for completion during class (10-15 min). These comprise approximately 10 short answer questions based on recent class material and reading assignments.

The Computational Mini-Project will involve building, optimizing, and analyzing a molecular structure in QChem. Each student will be assigned a different molecule. Students will run a series of calculations on their molecule to extract specific property values. These values will be combined with data from the rest of the class and analyzed to explore possible trends within the group of molecules studied. Students will be assessed on the accuracy of their results compared to those obtained from similar experiments performed by the instructor.

The Database Project will serve as a real-world test of course material. Students will be tasked with reading and extracting key information from recently published papers in the field of molecular electronics. Work will be graded on accuracy and completeness. The extracted data will be uploaded to a new databased-based literature search tool under developement by Prof. Inkpen (the *Molecular Junction Database*), making it available for use by active researchers in the field of Molecular Electronics. Each student will be assigned ~10 recently published papers to read and index outside of class time. Questions and additional parameters for this assignment will be posted after the mid-term.

The Final Exam is a ~1 h closed book written examination where students will be expected to answer questions based on the class material and reading assignments.

Grading Breakdown

Assessment Tool (assignments)	Due	% of Grade
"Poll Everywhere" questions	Each Class	5 (participation only)
3 x In-class pop quiz	Weeks 2, 4, 6	10 (total)
Computational mini-project	Week 3/4	5
Database project	April 29	40
Final exam	May 8 (tentative)	40
TOTAL		**100**

No make-up exams can be given. Absences will be excused only for medical reasons or in the case of extreme necessity. No "doctors note"/student health center slips are required, but absences may only be authorized by giving *advance* notice to the instructor. In the case of an excused absence, a grade will be assigned which is based on the average of the students class rank on their other graded material. Any unauthorized absence will result in a grade of zero for that exam. Requests for regrading of any exam/project work must be submitted within one week after the graded material is made available to you. Graded material will be photocopied before redistribution. A request for regrading of an altered exam is a serious violation of academic integrity.

Assignment Submission Policy

Assignments should be submitted electronically (through email/Blackboard/TurnItIn as directed) by 5 pm on the specified date.

Grading Timeline

The instructor aims to grade and provide feedback for all assessments within 1 week of submission.

Additional Policies

Students are expected to attend all in-person lectures and participate in class discussions. The use of laptops and other electronic devices during lectures for class-related web searches or calculations is encouraged, so long as their use is not disruptive to the rest of the class.

Practical Demo: Scanning Tunneling Microscope-based Break Junction

Students can schedule an *optional, ungraded* lab session (3-4 h) to run a single-molecule conductance experiment using the scanning tunnelling microscope-based break junction method (with a state-of-the-art instrument that is in active use within the Inkpen Lab). They can choose from a selection of stock molecules, a commercially available molecule of their choice, or measure a molecule they have independently obtained (e.g., through synthesis in their own research lab).

University Holidays/Event Conflicts (no classes on these dates)

March 17 – Spring Recess
March 20 – Spring Recess
April 14 – Passover
April 24 – Stauffer Symposium
April 28 – No Class

Course Schedule: A Weekly Breakdown

An outline of the topics to be covered is provided below (exact topics and dates are subject to change). To reinforce and expand upon class concepts, additional readings (2-3 papers/excerpts) per class will be assigned from seminal or recent primary and secondary literature publications.

Class	Readings/Preparation	Topic	Deliverables
1	*Nat. Nanotechnol.*, 2013, **8**, 378	Introduction to Molecular-Scale Electronics, Why Study Molecular-Scale Electronics Today?	
2	Schedule Measurement Demo	Single-Molecule Measurement Techniques Large Area Measurement Techniques	
3	Run assigned lit. searches	Building the Molecular Junction Database	
4	Watch "Datta" Lecture(s)	Fundamental Charge Transport Theory Fundamental Charge Transport Theory (cont.)	Pop Quiz
5	*Mater. Horiz.*, 2014, **1**, 17	Energy Level Alignment, Interface Effects HOMO-LUMO gaps	
6		Introduction to Computational Methods Basic Applied Computational Methods	
7	Run assigned calculation(s)	Basic Applied Computational Methods (cont.) Electrode Linker Groups	
8	*Nanoscale*, 2021, **13**, 1103 "Curly Arrow" practice set	π-, Homo-, Cross-Conjugation Quantum Interference Effects	Pop Quiz
9		Thermoelectricity Electrochemistry	
10		Non-Covalent Interactions Biochemical Systems (DNA, peptides, etc)	
11		*Devices I:* Switches *Devices II:* Diodes	
12	*Nat. Nanotechnol.*, 2013, **8**, 385	Non-Au Electrode Materials Special Topics/Future Directions/Challenges	Pop Quiz
Ad Hoc – Practical Demo: Scanning Tunneling Microscope-based Break Junction			
April 29 – Database Project DUE			
May 8 (tentative) – **FINAL EXAM** (All Materials)			

Statement on University Academic and Support Systems

Students and Disability Accommodations:
USC welcomes students with disabilities into all of the University's educational programs. The Office of Student Accessibility Services (OSAS) is responsible for the determination of appropriate accommodations for students who encounter disability-related barriers. Once a student has completed the OSAS process (registration, initial appointment, and submitted documentation) and accommodations are determined to be reasonable and appropriate, a Letter of Accommodation (LOA) will be available to generate for each course. The LOA must be given to each course instructor by the student and followed up with a discussion. This should be done as early in the semester as possible as accommodations are not retroactive. More information can be found at osas.usc.edu. You may contact OSAS at (213) 740-0776 or via email at osasfrontdesk@usc.edu.

Student Financial Aid and Satisfactory Academic Progress:
To be eligible for certain kinds of financial aid, students are required to maintain Satisfactory Academic Progress (SAP) toward their degree objectives. Visit the Financial Aid Office webpage for undergraduate- and graduate-level SAP eligibility requirements and the appeals process.

Support Systems:
Counseling and Mental Health - (213) 740-9355 – 24/7 on call
Free and confidential mental health treatment for students, including short-term psychotherapy, group counseling, stress fitness workshops, and crisis intervention.

988 Suicide and Crisis Lifeline - 988 for both calls and text messages – 24/7 on call
The 988 Suicide and Crisis Lifeline (formerly known as the National Suicide Prevention Lifeline) provides free and confidential emotional support to people in suicidal crisis or emotional distress 24 hours a day, 7 days a week, across the United States. The Lifeline consists of a national network of over 200 local crisis centers, combining custom local care and resources with national standards and best practices. The new, shorter phone number makes it easier for people to remember and access mental health crisis services (though the previous 1 (800) 273-8255 number will continue to function indefinitely) and represents a continued commitment to those in crisis.

Relationship and Sexual Violence Prevention Services (RSVP) - (213) 740-9355(WELL) – 24/7 on call
Free and confidential therapy services, workshops, and training for situations related to gender- and power-based harm (including sexual assault, intimate partner violence, and stalking).

Office for Equity, Equal Opportunity, and Title IX (EEO-TIX) - (213) 740-5086
Information about how to get help or help someone affected by harassment or discrimination, rights of protected classes, reporting options, and additional resources for students, faculty, staff, visitors, and applicants.

Reporting Incidents of Bias or Harassment - (213) 740-2500
Avenue to report incidents of bias, hate crimes, and microaggressions to the Office for Equity, Equal Opportunity, and Title for appropriate investigation, supportive measures, and response.

The Office of Student Accessibility Services (OSAS) - (213) 740-0776
OSAS ensures equal access for students with disabilities through providing academic accommodations and auxiliary aids in accordance with federal laws and university policy.

USC Campus Support and Intervention - (213) 740-0411
Assists students and families in resolving complex personal, financial, and academic issues adversely affecting their success as a student.

Diversity, Equity and Inclusion - (213) 740-2101
Information on events, programs and training, the Provost's Diversity and Inclusion Council, Diversity Liaisons for each academic school, chronology, participation, and various resources for students.

USC Emergency - UPC: (213) 740-4321, HSC: (323) 442-1000 – 24/7 on call
Emergency assistance and avenue to report a crime. Latest updates regarding safety, including ways in which instruction will be continued if an officially declared emergency makes travel to campus infeasible.

USC Department of Public Safety - UPC: (213) 740-6000, HSC: (323) 442-1200 – 24/7 on call
Non-emergency assistance or information.

Office of the Ombuds - (213) 821-9556 (UPC) / (323-442-0382 (HSC)
A safe and confidential place to share your USC-related issues with a University Ombuds who will work with you to explore options or paths to manage your concern.

Occupational Therapy Faculty Practice - (323) 442-2850 or otfp@med.usc.edu
Confidential Lifestyle Redesign services for USC students to support health promoting habits and routines that enhance quality of life and academic performance.