Graduate Evening Courses in Chemistry, Fall 2022:
COMPUTATIONAL • ORGANIC • ANALYTICAL

- The Chemistry Department at Rutgers Newark (http://sasn.rutgers.edu/chemistry) will offer Graduate Courses in Physical Chemistry, Organic Chemistry, Analytical Chemistry in Fall 2022.
- **When/where:** Courses will be held in Smith and Engelhard Hall once a week from 6:00 PM to 9:00 PM
- Register [HERE](http://sasn.rutgers.edu/chemistry) or scan the code

**Computational Chemistry (26:160:529)**
**MONDAYS 6:00 - 9:00 PM**
Engelhard Hall Room 215

**Instructor:** Prof. Michele Pavanello  
**Email:** M.PAVANELLO@RUTGERS.EDU

The goal of this 3-credit course for Chemistry, Physics and Materials science students is to provide basic knowledge of the theory of materials science and molecular quantum mechanics when it is applied to determine properties (e.g., photoelectron spectroscopy, IR, UV/Vis, NMR, etc...) as well as chemical reactivity and dynamics. Lectures will be divided in two parts: The first part (1.5 hours) will be devoted to the study of theoretical tools at the foundation of quantum chemistry and quantum materials science. The second part of the lectures will be devoted to practical applications of the concepts learned during the first part of the lecture and will involve Python coding or training on the use of off-the-shelf electronic structure software. Concepts touched will range from linear algebra, Hartree-Fock and DFT methods to correlated wavefunction methods. Practical use of these concepts with Quantum ESPRESSO, Gaussian, Psi4 and PySCF on systems and processes useful to the students and their advisors will constitute a substantial part of the class effort.

**Chemistry of Heterocyclic Compounds (26:160:501)**
**WEDNESDAYS 6:00 - 9:00 PM**
Smith Hall Room 240

**Instructor:** Prof. Michal Szostak  
**Email:** MICHAL.SZOSTAK@RUTGERS.EDU

This course will cover fundamental principles and advanced topics in heterocyclic chemistry. Synthesis and reactivity of major classes of heterocyclic compounds are covered in detail, with emphasis on recent advances in synthesis and reaction development. Special attention is given to heterocycles of biological interest and the importance of heterocycles in the pharmaceutical industry, including pyrroles, furans, thiophenes, indoles, quinolines, oxazoles, imidazoles, triazoles and aziridines. Special focus is placed on critical evaluation of heterocyclic chemical literature, presentation of seminars and short reviews in heterocyclic chemistry. Each student will be asked to present a short seminar (20-30 min) based on an original research paper from the current heterocyclic literature and present short “Spotlight” reviews (5 min) on research papers on a popular heterocycle from the current heterocyclic chemistry literature.

**Electroanalytical Chemistry (26:160:549)**
**THURSDAYS 6:00 - 9:00 PM**
Smith Hall Room 240

**Instructor:** Prof. Huixin He  
**Email:** HUIXINHE@NEWARK.RUTGERS.EDU

This course introduces the fundamentals of electrochemistry and commonly used electro-analytical methods, such as cyclic voltammetry, linear sweep voltammetry with rotating disk-ring electrodes, stripping voltammetry, the unique electrochemical behavior of micro/nanoelectrodes, pulse voltammetry techniques, and AC impedance spectroscopy, and scanning electrochemical microscopy techniques. Frontier research in various fields using these electrochemical techniques will be discussed. Each student will be asked to present a short seminar on how electrochemical techniques are used in various research fields.