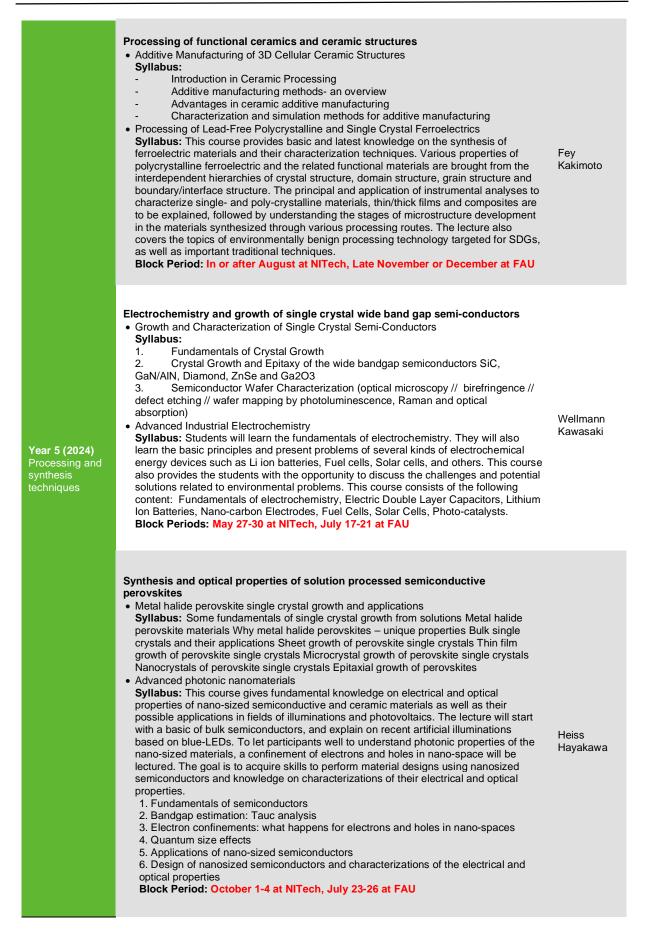
Lecture Outline and Schedule

| Year | Module | Lecturer |
|---|--|--------------------|
| Year 4 (2023) Introduction of the material classes and modeling techniques | Introduction to lead-free perovskite ferroelectrics for electro-mechanical systems Mechanical Properties of Ferroelectrics Syllabus: This lecture is an introduction to dielectric, piezoelectric, and ferroelectric properties of ferroelectrics. In the first section, background on dielectric and piezoelectric properties will be discussed with a focus on the influence of material phenomena at multiple length scales, such as domain wall and phase boundary motion, as well as the influence of external thermal, mechanical, and electric fields. Various measurement techniques, such as Rayleigh behavior and impedance spectroscopy, will be introduced. In the second section, the large field response of ferroelectrics, namely ferroelectricity and ferroelasticity will be discussed with a particular focus on the effect of crystal structure and compositional phase boundaries, the role of domain wall motion and defects, and the influence of stress-induced structural phase transformations. Measurement techniques for characterizing large field behavior, such as the Sawyer-Tower circuit, will also be introduced. Following this lecture it is expected that the participant is familiar with the dielectric, piezoelectric, and ferroelectric properties of normal ferroelectrics Syllabus: This course provides basic and latest information on the functional properties of ferroelectric materials, in which the orientation of spontaneous polarization changes with electric field, stress or temperature. In the first section, an introduction of this course deals with the crystal chemistry of ferroelectric materials and differences in history and characteristics among lead-free based materials including (Na,K)NbO₃, (Ba,Ca)(Ti,Zr)O₃, (Na,Bi)TiO₃, BiFeO₃ perovskites and their relative compounds. In the third and fourth sections, the lecture is extended to cover the topics of important ferroelectric families including piezoelectric which are polarization thermals including piezoelectrics which | Webber Kakimoto |
| | Materials and devices for opto-electric and energy technologies NGSE5 Seminar Syllabus: 10 Tutorials (each 1h) will be given to acquire theoretical foundations, followed by a debriefing for questions of students. Supplementary 15 keynote speeches (each 15min) on highly topical issues will be held: 6 presentations on a timely OPV topic, 6 on a timely perovskite topic and 3 on a timely emerging PV topic. Electronic Materials Analysis Syllabus: This lecture introduces theory and practice of electronic materials characterization and analysis based on the case of semiconductors. Characterization and analysis techniques for semiconductors can easily be applied to other electronic materials. A textbook of the lecture will be "Semiconductor Material and Device Characterization" by Schroder, D. Wiley-IEEE Press, c2006 | Brabec Kato |
| | Introduction to atomistic and mesoscale modeling • Electro-Mechanical-Modeling(EMM) Syllabus: This course will cover the following topics: Tensor Calculus • Continuum Mechanics • Electro-Magneto-Dynamics • Electro-Statics • Electro-Statics • Electro-Mechano-Statics • Electro-Mechano-FEM • Simulation for Nano-Technology Syllabus: This course will cover the following topics related to the molecular dynamics simulation: • Empirical Inter-atomic Potentials • Time-evolution Algorithms • Long-ranged Coulomb Interaction • Essential Techniques • Recent Results Block Periods: TBD at NITech, November 6-10,2023 at FAU | Steinmann Ogata |



Nanostructured surfaces

• Modeling of Surface Phenomena

Syllabus: The lecture starts with a brief introduction into quantum-chemical methods for surface science studies. Important practical issues when performing calculations are addressed. In the next section, the basic nomenclature of how to describe the atomic and electronic structure of surfaces is introduced. Basic concepts on how to understand the electronic properties of metal, semiconductor and insulator surfaces, such as surface states, dangling bonds, passivation, charge neutralization with respect to polar and nonpolar surfaces will be explained. This will be combined with a thermodynamic analysis of the stability of surface structures, which will allow to derive surface phase diagrams. These concepts will be used to understand adsorption properties and surface chemical reactions. Finally, methods for calculating STM and AFM data to support the analysis of experimental data from local probe measurements are discussed.

Ceramics Interface Chemistry

Syllabus: Ceramics materials, which are representative of the oxide, are complexed with other oxides or metals to improve the surface/interface properties. This lecture provides the physico-chemical properties and their characterization techniques of ceramics interface at which various physical and chemical phenomena such as molecular adsorption, catalysis, electron transfer etc. take place. Students will learn the foundation and application of surface/interface chemistry occurred on advanced ceramics materials, mainly focusing on catalyst.

Block Periods: November 27-December 1,2023 at NITech, TBD at FAU.

Meyer Haneda

Advanced structural characterization techniques

Vibrational Spectroscopy of Amorphous To Nucleated To Fully Crystallized Materials

Syllabus: This lecture introduces theory and practice of Vibrational Spectroscopy techniques. Students will learn the fundamentals, the instrumentation, and the challenges in data acquisition/interpretation. Therefore, Hands-on training sessions are planned.

- Basic theory and fundamentals;

Year 6 (2025)

development

and advanced

Device

- Raman and FTIR spectrometers;
- Applications & Complementary techniques
- PRACTICE: Sample preparation & measurements (if allowed)
- PRACTICE: Data handling: from calibration to data presentation
 - PRACTICE: Interpretation: quantitative vs qualitative

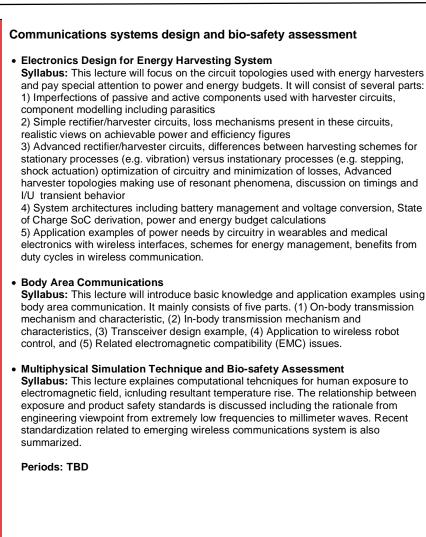
• Synchrotron Radiation Techniques for Materials Science

Syllabus: This lecture introduces materials characterization techniques using synchrotron radiation, which produce strong and energy tunable X-rays. Unlike ordinary X-ray analyses, students will learn how powerful synchrotron-based X-ray techniques for element-selective structural analyses.

- Basics of Synchrotron Radiation;
- Introductions of Various Synchrotron-Based X-ray Techniques;
- X-ray Absorption Fine Structure (XAFS)
- X-ray Fluorescence Holography (XFH)

Block Periods: TBD

Cicconi Hayashi



Advanced modeling techniques for mechano-electrical systems

Modeling and Simulation of Piezo-Electric Energy Harvesters

Syllabus: The course provides an overview of modeling and simulation approaches for piezoelectric energy harvesters. In the first part of the course, there is a short introduction about the applications of piezoelectric energy harvesters. Then, the basic equations of electro-mechanical models are derived, both for linear and nonlinear material behavior. Building on these continuous equations, the simulation of piezoelectric structures using the finite element method is shown. This is followed by a discussion of the simulation of electric circuits and their coupling with electromechanical structures. Examples of linear energy harvesters and their dynamic simulation using harmonic response analysis follow. In the last part of the course, the coupled simulation of nonlinear energy harvesters with nonlinear circuits is discussed.

Advanced Lecture on Motor Drives

Syllabus: In recent years, an electric and a fuel cell vehicle have been put to practical use in the market for a demand of CO2 emission reduction for protecting global warming. These kinds of vehicles employ electric motor drives for their propulsion. This lecture provides explanations about various types of the electric motors and their working principles, drive methods based on power electronics and aspects from a viewpoint of the vibration that is a dominant source of noise to be suppressed by piezo-actuated shape-adaptive structures as well as gives us an opportunity of developing piezo-actuated energy harvesting system.

Block Periods: TBD

Fischer Anzai

Mergheim Kosaka

Crystal growth and material processing - experimental and numerical approaches

Introduction to the phase-field method for crystal growth, processing and multiferroics

Syllabus: This lecture introduces the key ingredients to understand and implement the phase-field method (PFM), which has established as an important simulation tool to understand mesoscopic structure evolution in alloys, ceramics and soft matter. In the course the focus lies on applications in crystal growth, solidification and thin film growth of multi-component systems (alloys and minerals), but we will also touch domain or variant evolution in multiferroic systems, such as ferroelectrics, shape memory alloys (SMAs) and ferromagnetic SMAs.

The basic idea of introducing diffuse interfaces that simplify the numerical treatment of this kind of free boundary value problems is explained, and the mathematical and physical background including thermodynamics is developed. A lecture of its own will be dedicated to implementation of this method, including feasible and flexible software packages that can be used without long-standing experience in numerics. From elementary description of interfacial phenomena to the kinetics of crystalline interfaces, increasingly complex models including single phase-field to multiple phase-field methods are exploited. Important transport processes containing diffusion, fluid flow and mechanical deformation are coupled. The goal is to convey a tool to study intricate pattern formation during solidification (dendrites), eutectic lamellae growth,

flow and mechanical deformation are coupled. The goal is to convey a tool to study intricate pattern formation during solidification (dendrites), eutectic lamellae growth, precipitate growth and solutal crystal growth. Additional chapters on the relationship of PFM to atomistic simulation techniques (MD, DFT) will be presented, allowing for a length scales bridging in computational modeling.

• Crystal growth of semiconductor and material processing using ultrashort laser pulses

Syllabus: This course provides basic and latest knowledge on the crystal growth of semiconductor materials, especially about epitaxial growth. This course also provides the latest fine processing technique using ultrashort pulse lasers.

Block Periods: TBD

Wendler Miyagawa