# Formato para registro de Unidades de aprendizaje

## I.- Datos de identificación de la Unidad de aprendizaje

| | |
|---|---|
| Unidad académica: | Centro Interdisciplinario de Investigaciones y Estudios sobre Medio Ambiente y Desarrollo |
| Nombre del Programa académico: | Doctorado en Ciencias en Estudios Ambientales y de la Sustentabilidad |
| Grado | Doctorado |
| Orientación | Científica |
| Sesión de colegio donde se propuso: | VIII REUNIÓN ORDINARIA DEL COLEGIO DE PROFESORES |
| Fecha de propuesta: | 18/06/2024 |

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|---|---|
| Nombre de unidad de aprendizaje: | **Thermodynamics and Physicochemical Phenomena of an Electrochemical System** |
| Clave de la unidad de aprendizaje: | 24B9030 |
| Créditos: | 5 *REP 2017* |
| Semanas por semestre | 18 |
| Horas a la semana: | 4 |
| Horas totales: | 72 |
| Tipo de unidad de aprendizaje: Obligatoria: | ☐ |
| Optativa: | ☒ |
| Semestre: | -- |
| Observaciones: | This unit needs an entry profile with a firm grasp of general physics, chemistry, and thermodynamics. |

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|---|---|
| Área del conocimiento: | Ingeniería y Ciencias Fisico Matemáticas |

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**II. Aprendizajes que, al finalizar, el estudiantado deberá demostrar**

| Conocimientos | Habilidades y destrezas | Actitudes y valores |
|---|---|---|
| • Overview of electrochemistry, fundamentals of electricity, and electrolyte solutions.<br>• Students should grasp the concept of chemical potential in chemical reactions, Gibbs free energy, the concepts of activity and fugacity, applied to chemical equilibrium in electrochemical reactions.<br>• They should be able to classify galvanic and electrolytic cells, understand electrochemical potential and apply the Nernst equation. Additionally, they must comprehend and apply the absolute electrode potential scale, and its importance in electrochemistry.<br>• Deduct and apply the Butler-Volmer and Tafel equations to understand experimental current-potential responses.<br>• Understand the Marcus-Gerischer kinetic models for outer-sphere reactions and estimates for inner-sphere reactions.<br>• How to operate electrochemical instruments such as potentiostats/galvanostats and understand the experimental aspects of three-electrode systems and reference electrodes.<br>• Apply basic electrochemical methods for AC and DC, including electrochemical | • How to solve problems related with the analysis and understanding of the electrical conductivity of electrolyte solutions.<br>• Explain clearly and concisely complex electrochemical concepts to both specialized and non-specialized audiences.<br>• Calculate the thermodynamic properties of chemical reactions and electrochemical systems.<br>• How to use Nernst's equation and other relevant equations to solve electrochemical equilibrium problems.<br>• Deduct and apply kinetic equations such as Butler-Volmer and Tafel to analyze electrochemical reactions.<br>• Explain and analyze interfacial phenomena using advanced theories and models such as the Marcus-Gerischer model.<br>• How to operate electrochemical instruments such as potentiostats and galvanostats and set up three-electrode experimental systems.<br>• Interpret spectra and graphs, such as impedance spectra and Nyquist plots, to characterize the electrochemical properties of materials. | • Understand and explain the underlying phenomena in charge transfer at electrochemical interfaces.<br>• Appreciate the precision in calculations and results, recognizing the importance of rational use of the involved equations.<br>• Promote collaboration in environmental application projects, acknowledging the interdisciplinary nature of electrochemical science in this field.<br>• Encourage the ability to address ecological challenges innovatively and creatively, applying electrochemical methods to practical ecosystem treatment situations.<br>• Promote critical thinking to constructively evaluate and question models and obtained results.<br>• Foster the ability to critically analyze relevant scientific literature on the subject. |

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| impedance spectroscopy, voltammetry, chronopotentiometry, and potentiometry.<br>• Perform physicochemical characterization of materials using techniques such as UV-Vis spectroscopy, TEM analysis, Debye function analysis, among others.<br>• Recognize the importance of electrochemistry in studying and addressing environmental pollution phenomena. | | |

*Resolución que aborda la propuesta con su enfoque disciplinar*

Este rubro debe centrarse en los aspectos que resuelven o indagan la(s) disciplina(s) o tema(s) que se aborda(n), tome en cuenta que no se desea registrar aquí el estado del arte que guarda un conocimiento acumulado dentro de un área específica, sino la respuesta que se da con esta planeación didáctica ante una problemática definida.

In the study, research, and application of environmental remediation procedures, the tools provided by electrochemistry are fundamental. The increasing availability of potentiostats-galvanostats for three-electrode systems and power sources for two-electrode cells at more affordable costs has increased the availability of these tools. They are becoming increasingly accessible to professionals and small to medium-sized enterprises in both the public and private sectors. For this reason, the *"Doctorado en Ciencias en Estudios Ambientales y de la Sustentabilidad"* program needs to integrate this knowledge into its academic curriculum, which it currently does not. These tools have become indispensable for understanding the phenomena of generation and treatment of atmospheric, aquatic, and biological contaminants.

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Secretaría de Investigación y Posgrado
Dirección de Posgrado

SIP-30
2024

**F o r m a t o  p a r a  r e g i s t r o  d e  U n i d a d e s  d e  a p r e n d i z a j e**

## III. Proximidad formativa

| *Áreas multi, inter y transdisciplinarias:* | *Líneas de Generación y Aplicación de Conocimiento:* | *Sectores sociales:* |
|---|---|---|
| Anote las disciplinas con las que se relacionan los temas de estudio de esta planeación. Tome en cuenta que su registro estará justificado si contempla información efectiva (y evidente) para el aprendizaje propuesto. | Se retoman del programa académico según corresponda. | Sectores sociales donde puedan promoverse los productos académicos que resultan del natural ejercicio formativo que se está planificando. Enuncie los sectores o grupos que consideres viables. |
| • General chemistry.<br>• Analytical chemistry.<br>• Differential equations.<br>• Numerical methods.<br>• Environmental engineering.<br>• Catalysis. | • Atmospheric pollutant emissions and their implications on air quality.<br>• New materials for low sulphur fuel production and absorbents for pollution reduction.<br>• Urban and hazardous solid waste management. | •Academia and Research.<br>•Industry.<br>•Governmental Sector. |

*E s t r a t e g i a  d e  a s o c i a c i ó n :*

Integre sintéticamente las consideraciones para delimitar cómo interactúa el estudiante con los sectores de la sociedad (previamente considerados) en función de la mediación de conocimientos que se pretende abordar y los aspectos que resuelve o indaga.

• Academia and Research: Publication in academic journals, conference presentations and participation in scientific events to share knowledge with the academic community.
• Industry: Collaboration with companies in the chemical, pharmaceutical, food, and other sectors to apply the acquired knowledge in the course to practical problems and industrial developments.
• Government Sector: Collaboration with government entities related to regulation, environment, health, among others, to provide advice on decisions based on the reinforcement of knowledge obtained through electrochemical techniques.

## IV. Contenido temático (incluya el tiempo requerido si lo considera apropiado)

**1. Course Content**

**2. Course Evaluation**

**3. Units**

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**UNIT 1: Fundamentals of Electrolyte Solutions**

1.1 A summary of electrochemistry
  1.1.1 A Brief Summary of Electrochemistry
  1.1.2 Definition of Electrochemistry
1.2 Basic concepts
  1.2.1 Electricity
  1.2.2 Electric field geometries
  1.2.3 Materials classification based on electrical conductivity
1.3 Electrolyte solutions
  1.3.1 Conductor classification
    1.3.1.1 Electrolyte and non-electrolyte classification
    1.3.1.2 Electronic conductors
  1.3.2 Electrical conductivity in electrolyte solutions
    1.3.2.1 Ionic conductors
    1.3.2.2 Kohlrausch's Law
  1.3.3 Debye-Hückel Theory of Electrolyte Solutions

**UNIT 2: Chemical Equilibrium in Electrochemical Reactions**

2.1 Chemical potential in chemical reactions

  2.1.2 Gibbs energy free in gas phase
  2.1.3 Activity and fugacity
  2.1.4 Thermochemistry
  2.1.5 Thermal equilibrium
  2.1.6 Equilibrium criteria
  2.1.7 Activity and fugacity in gas and liquid phases
  2.1.8 Arrhenius' equation
  2.1.9 Kirchhoff's equation or Kirchhoff's law

2.2 Chemical potential of electrolytic solutions
  2.2.1 Convention I and II for standard states
  2.2.2 Thermodynamic properties of non-ideally dilute solutions
  2.2.3 Example calculations
  2.2.4 Mean chemical potential, ionic activity coefficient, and mean ionic concentration

2.3 Classifications of Electrochemical Systems
- 2.3.1 Galvanic cell
- 2.3.2 Electrolytic cell
- 2.3.3 Types of electrochemical systems

2.4 Thermodynamics of Electrochemical Systems
- 2.4.1 Electrochemical potential
  - 2.4.1.1 Outer potential or Volta potential ($\psi$)
  - 2.4.1.2 Surface potential ($\chi$)
  - 2.4.1.3 Inner potential or Galvani potential ($\phi$)
  - 2.4.1.4 Chemical potential ($\mu^{a}_{i}$) and its physical and thermodynamic definitions
  - 2.4.1.5 Electrochemical potential and related work functions
  - 2.4.1.6 Nernst equation from electrochemical potentials
  - 2.4.1.7 Ab-initio calculation of reduction potentials
  - 2.4.1.8 Calculation of $\Delta U$ and $\Delta G$ for specific cell reactions
  - 2.4.1.9 Electric work and first law of thermodynamics
- 2.4.2 Electrochemical Reaction Equilibrium
  - 2.4.2.1 Gibbs-Duhem's Equation and Electrochemical Reaction Equilibrium
  - 2.4.2.2 Electrochemical potential and equilibrium conditions
  - 2.4.2.3 Electromotive force (emf) and its operational definition
  - 2.4.2.4 Electrochemical electromotive series and standard potentials
  - 2.4.2.5 Calculation from thermodynamic properties of reactions
  - 2.4.2.6 Nernst equation
  - 2.4.2.7 Construction and interpretation of Latimer and Frost diagrams
- 2.4.3 Absolute Electrode Potential Scale
  - 2.4.3.1 Single electrode Potential
  - 2.4.3.2 Absolute Electrode Potential
  - 2.4.3.3 Standard Hydrogen Electrode Potential
  - 2.4.3.4 Absolute Reduction Potential Table
- 2.4.4 Applications of Nernst equation
  - 2.4.4.1 Common cells in electrochemistry

**UNIT 3: Faraday's law of electrolysis and Electrochemical Kinetics**

3.1 Faraday's law of electrolysis
- 3.1.1 Faraday's law of electrolysis
- 3.1.2 Equivalent circuits
- 3.1.3 Ideal polarizable electrode

3.2 Electrochemical Kinetics
- 3.2.1 Electrical Double Layer
  - 3.2.1.1 Electron Transfer Mechanisms "Marcus' Theory"
  - 3.2.1.2 Nernst-Planck equation
  - 3.2.1.3 Interfacial phenomenon
- 3.2.2 Butler-Volmer equation
  - 3.2.2.1 Butler-Volmer derivation
  - 3.2.2.2 Tafel equation
  - 3.2.2.3 Hydrogen evolution reaction
- 3.2.3 Kinetic models Marcus-Gerischer
  - 3.2.3.1 Outher Sphere Reactions Marcus Model
  - 3.2.3.2 Reorganization Energy
  - 3.2.3.3 Charge Transfer coefficient
  - 3.2.3.4 Activation Energy – Reorganization Energy
  - 3.2.3.5 Solid State Model
  - 3.2.3.6 Fermi-Dirac distribution
  - 3.2.3.7 Gerischer model
  - 3.2.3.8 Probability Density Function
  - 3.2.3.9 Gerischer – Marcus Model

**UNIT 4: Electrochemical methods**

4.1 Electrochemical instruments
- 4.1.1 Potentiostat/Galvanostat
- 4.1.2 Experimental aspects
  - 4.1.2.1 Three electrode system
  - 4.1.2.2 Reference electrode

4.2 Basic Electrochemical methods
- 4.2.1 AC and DC methods
  - 4.2.1.1 Electrochemical Impedance Spectroscopy
  - 4.2.1.2 Voltammetry
  - 4.2.1.3 Chronoamperometry
  - 4.2.1.4 Potentiometry
- 4.2.2 Electroanalytical methods
  - 4.2.2.1 Voltammetry
  - 4.2.2.2 Potentiometry
  - 4.2.2.3 Coulometry

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4.3 Selected topics in Electrochemistry and its applications
- 4.3.1 Physicochemical characterization
  - 4.3.1.1 Derivative peak-fitting of diffuse reflectance UV-Vis spectra (DPR) Derivative peak-fitting of diffuse reflectance UV–Vis spectra (DPR)
  - 4.3.1.2 Electrochemical Impedance Spectroscopy: Fundamentals and applications
  - 4.3.1.3 TEM analysis
  - 4.3.1.4 XRD: Debye Function analysis
  - 4.3.1.5 Surface electrochemical analysis
  - 4.3.1.6 Probing electronic centers
- 4.3.2 Electrochemical Energy Source
  - 4.3.2.1 Fuel cell reactions
  - 4.3.2.2 Catalytic effect vs. structural properties
  - 4.3.2.3 Interaction energy DFT-Calculation
- 4.3.3 Environmental remediation with Electrochemical Technologies
  - 4.3.3.1 Emerging Pollutants
  - 4.3.3.2 Design of electrochemical reactors
  - 4.3.3.3 Electrocoagulation
  - 4.3.3.4 Microbial Fuel Cells
- 4.3.4 Corrosion
  - 4.3.4.1 Fundamentals and kinetics of corrosion
  - 4.3.4.2 Corrosion types
  - 4.3.4.3 Beneficial aspect of corrosion
  - 4.3.4.4 Selected topics in corrosion science

**Experimental Electrochemistry**

Practice No 1: Construction of a reference electrode

Practice No. 2 Cyclic Voltammetry as a tool to characterize a solid electrode

Practice No. 3 Determination of electrons in a reaction from Electrode disk rotatory technique

Practice No. 4 Characterization of RC circuit from electrochemical impedance spectroscopy technique.

Practice No. 5. Determination of corrosion rate by weight-loss method

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## V. Referencias

| Documentales / electrónicas |
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3. R. Chang, K. Goldsby, *Chemistry*, McGraw Hill Education, USA, 2016.
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5. K.B. Oldham, J.C. Myland, A.M. Bond, *Electrochemical Science and Technology: Fundamentals and applications*; John Wiley & Sons, Ltd, Publications: 2011.
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8. I.N. Levine, *Physical Chemistry*, 6th ed., Mc Graw Hill Higher Education, New York, USA, 2009.
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20. Alonso-Vante, N. *Chalcogenide Materials for Energy Conversion*; Springer International Publishing AG: Cham, 2018.

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## VI. Evaluación

Three theoretical exams: 40%
Assessment of theoretical knowledge through written exams covering the fundamentals of electrochemical techniques.

Four laboratory sessions: 30%
Assessment of practical skills and the ability to apply knowledge to their master's thesis topics in the laboratory.

Class participation and discussions: 20%
Continuous assessment of participation in classes, discussions, and critical analysis of results obtained in the laboratory and in model problems.

Presentation of application to specific thesis topic: 10%
Since computational modelling will be applied by each student to their master's thesis topic, the results can be presented in class and in the corresponding thesis, thereby contributing to strengthening the findings and the proponent's curriculum.

## VII. Créditos y responsivas

| Responsabilidad | Nombre completo | Clave de nombramiento |
|---|---|---|
| Coordinador (Autor) | Dr. Luis Alberto Estudillo Wong | 15983-EB-22 |
| Participante (Coautor) | Dr. Raciel Jaimes López | 17968-EA-24 |
| Participante (Coautor) | Dr. Juan Alberto Alcántara Cárdenas | 17092-EA-23 |

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