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<tr><td>Course Code</td><td colspan="2">CHE404M3</td></tr>
<tr><td>Course Title</td><td colspan="2">Advanced Topics in Statistical Thermodynamics and Electrochemistry</td></tr>
<tr><td>Credit Value</td><td colspan="2">3</td></tr>
<tr><td rowspan="2">Hourly breakdown</td><td>Theory</td><td>Independent learning</td></tr>
<tr><td>45</td><td>105</td></tr>
<tr><td>Objective/s</td><td colspan="2">
Provide the principals involved in relating the individual energy levels of atoms/molecules to the macroscopic thermodynamic properties and their application to simple systems.
Develop models for ion-ion and ion-solvent interactions
Discuss mathematical relationships related to the electrode/electrolyte interface
Explain equations for the rates of reactions that occur at the interface
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<tr><td>Intended Learning Outcomes</td><td colspan="2">
Calculate entropy of simple systems from the occupation of energy levels using the statistical definition of Entropy
Define ensemble and partition function
Relate partition function of an ideal gas to that of single atoms/molecules
Calculate the contributions of translational, rotational and vibrational motions and of electronic levels to the partition function
Determine Gibbs free energy and equilibrium constant using Statistical Mechanics
Apply Nernst equation to electrochemical systems
Explain the electrochemical double layer based on common models
Describe the difference between mass-transfer and electron-transfer controlled electrochemical processes
Apply voltammetric methods in electroanalysis
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<tr><td>Course Contents</td><td colspan="2">Advanced Statistical Thermodynamics

Statistical definition of entropy, Ensembles, Canonical partition function of a system of non-interacting particles, Canonical partition function of a pure gas, Boltzmann distribution law, Ideal diatomic and mono atomic gases, Polyatomic gases, Equilibrium constants, Entropy and the third law, Intermolecular forces, Fluids.

Advanced Electrochemistry

Electrochemical equilibrium, ion-solvent interactions, Debye-Huckel theory, electrode / electrolyte interface, electrocapillary equation, structure of the electrified interface, electrode kinetics, over potentials, mass-transfer and electron transfer controlled reactions, Butler-Volmer equation, ion conducting and electronically conducting polymers, electrochemical methods
Voltammetry: Linear sweep voltammetry, cyclic voltammetry, differential pulse voltammetry, square-wave voltammetry, stripping voltammetry
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<tr><td>Teaching and Learning Methods / Activities</td><td colspan="2">Lectures, tutorial discussion, small group assignment, home-work assignments, e-learning, online learning</td></tr>
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<tr><td rowspan="2">Evaluation/Assessment Strategy</td><td>In-course Assessment</td><td>End-of-course Examination</td></tr>
<tr><td>30 %</td><td>70 %</td></tr>
<tr><td>Recommended References</td><td colspan="2">1. Atkins, P., and de Paula, “Physical Chemistry”, 10th edition, Oxford University Press, 2014.
2. Atkins, P., and de Paula, “Elements of Physical Chemistry”, 4th edition, Oxford University Press, 2007.
3. Bard, A. J., and Faulkner, L. R., “Electrochemical Methods Fundamentals and Applications”, 2nd edition, John Wiley & Sons, Inc., 2001.
4. Compton, R. G., and Banks, C. E., “Understanding Voltammetry”, World Scientific Publishing Co. Pte. Ltd., 2007.
5. Dill, K. A., and Bromberg, S. Molecular Driving Forces: “Statistical Thermodynamics in Chemistry and Biology”, Garland Science, 2002.
6. Seddon, J. M., and Gale, D. G., “Thermodynamics and Statistical Mechanics, Royal Society of Chemistry”, 2001.
7. Gupta, M. C., “Statistical Thermodynamics”, 2nd Edition, New Age International Publishers, 2006.</td></tr>
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