

राष्ट्रीय प्रौद्योगिकी संस्थान जमशेदपुर

NATIONAL INSTITUTE OF TECHNOLOGY JAMSHEDPUR

CHG5111: Thermodynamics and Electrochemistry (4 credits: 3-1-0)

Classical Thermodynamics: Laws of thermodynamics, thermodynamic functions and their relationships, Gibbs-Helmholtz and Maxwell relations, Van't Hoff equation, criteria of spontaneity and equilibrium, evaluation of absolute entropies, partial molar properties, chemical potential and its variation with temperature & pressure, Fugacity.

Statistical Thermodynamics: Introduction: Concept of ensembles, partition functions and distributions, microcanonical, canonical and grand canonical ensembles, canonical and grand canonical partition functions, Boltzmann, Fermi-Dirac and Bose-Einstein distributions, Gibbs paradox and Sackur – Tetrode equation. Concept of thermal wavelength. molecular partition functions – translational, rotational, vibrational, electronic, nuclear, equipartition theorem and its validity. chemical potential and chemical equilibrium – Saha ionisation formula, system of interacting molecules – imperfect gas, specific heat of electron gas, Bose condensation, Liouville theorem and its consequences, its quantum version, formulation of quantum statistics – density matrix.

Electrochemistry: Ion transport in solution - migration, convection and diffusion - Fick's laws of diffusion conduction - influence of ionic atmosphere on the conductivity of electrolytes - the Debye-Huckel-Onsager equation for the equivalent conductivity of electrolytes, electrical double layer: theories of double-layer structure, diffuse-double-layer theory of Gouy and Chapman, the Stern model, polarization and overvoltage, current-potential relationship (derivation of Butler-Volmer and Tafel equations), electrochemical energy systems: secondary cells, fuel cells.

Text Books/References:

1. S. Glasstone, Thermodynamics for chemists, Affiliated East West Press, 1965.
2. Atkins, P.W. 'Physical Chemistry', 6th Edn., Oxford University Press, 1998.
3. J. O. M. Bockris and A. K. N. Reddy, Modern Electrochemistry, Plenum Press, 1970.
4. J. Rajaram & J. C. Kuriacose, Thermodynamics for Students of Chemistry, Shobanlal Nagin Chand Co, 1986
5. K. L. Kapoor, A Text Book of Physical Chemistry, Volumes 2 and 5, 3rd Edition, Macmillan India Ltd, 2004.