Homi Bhabha National Institute
(A Deemed to be University u/s 3 of UGC Act, MHRD & an Aided Institution of DAE)
Anushaktinagar, Mumbai – 400094

On-line Course on

Advanced Materials Chemistry

October 14, 2024 to December 23, 2024

Every Monday, Wednesday, and Friday

Time: 16:00 to 17:30 hrs

Course Director: Prof. A. K. Tyagi

Dean, HBNI

Email: deanhbni@hbni.ac.in, aktyagi@hbni.ac.in

Target students: Research scholars and faculty members

A: Preamble

Homi Bhabha National Institute (HBNI), a deemed to be University and grant in aid institute of the Department of Atomic Energy has ten constituent Institutions (CI) and one off-campus centre (OCC), which are engaged in fundamental and applied research in basic sciences, mathematics, and engineering sciences. The CI/OCC of the HBNI are engaged in cutting edge and frontline areas of research in different fields. The nature of research in today's times is largely multi-disciplinary and materials form an important component of many research areas across various discipline. This necessitates the knowledge of various aspects of materials chemistry for young researchers as well as faculty members. In view of this, HBNI is starting an online course on "Advanced Materials Chemistry" comprising of 30 lectures (90 minutes duration per lecture). This exhaustive course would cover a wide range of topics such as basics of materials chemistry, their characterisation, chemical and trace analysis of materials as well as functional materials for magnetic, energy applications and device applications. The course would also help the researchers to appreciate and understand a wide range of research that appears in journals in the field of materials across disciplines. The lectures will be delivered online by experts in the respective subject areas from Bhabha Atomic Research Centre and HBNI (using the Webex platform which will also be available on Youtube).

For any clarifications, please contact Dr. (Smt) Anshu Singhal, HBNI, Course coordinator (asinghal@hbni.ac.in).

B: Target Students

Target students for the proposed course are young researchers engaged in PhD and faculty members from different CI/OCI of HBNI as well as other universities.

C. Registration fee structure:

(1) For participants from DAE organisations which are CIs/OCC of HBNI: No registration fee

(2) For participants from DAE organisations that are not CIs/OCC of HBNI: Rs. 500/- (plus applicable taxes)

(3) Participants from non-DAE organisations: Rs. 1000/- (plus applicable taxes)

If the non-DAE candidate wishes to appear for evaluation exam and receive the credit certificate, an additional fee of Rs. 1000/- (plus taxes) would be charged.

D. Course structure: The course will be completed in 30 lectures of 90 minutes each. The course will be of 600 level and will be a **three-credit** course for the students for whom the enrolment date for the PhD programme is 01.08.2024, however, for the students for whom enrolment date for the PhD programme is prior to 01.08.2024 the course will have **six credits.**

S. No.	Topic	No. of lectures
1	General materials chemistry	7
2	Characterisation techniques	6
3	Chemical, major, trace and ultratrace analysis	6
4	Functional materials (Part I)	5
5	Functional materials (Part II)	6

There will be regular assignments and examinations for students who want to earn credit for the course. To earn the credit, the participant should attend more than 75 % of the lectures, and clear the examinations with more than 50% overall marks. Students desirous of participating in the course may please register on AnuVidhya website (www.AnuVidhya.in). Those who meet attendance requirements of 75% but do not take assignments and exam can be given participation certificate by HBNI.

Research scholars who want to earn credits for the course should submit nomination through

the Chairman, Doctoral Committee. The proforma of nomination form is enclosed.

E. Syllabus

(Number of lectures: 30; Duration: 90 Minutes; Number of credits: 3)

(a) General materials chemistry **[7 Lectures]**

Basic concepts: Crystalline and amorphous materials, chemical bonding and structure correlation, close packed structures, concept of bonding, co-ordination number, radius ratio rules, lattice energies, bond energies basic structure types, various silicate, phosphate and borate structures, complex oxides such as: perovskites, pyrochlores, spinels, brownmillerites, framework structure, structure of common nuclear materials (oxides, metallic, carbides), typical examples of structure-property correlation, unusual structures.

Other general aspects: Defects and defect equilibria, different classifications of defects, point/line/surface/volume defects with examples, techniques employed study defects, defects stabilized structures, solid solutions and their applications, phase transitions and their classifications, thermodynamic classification of phase transitions, martensitic phase transitions, defects induced phase transitions, concept of metastable phases.

Synthesis of advanced materials

General concepts, equipments/materials required with few typical examples, scope and limitations of different synthesis techniques: solid state synthesis, hydrothermal synthesis, ultrasonication and microwave synthesis, metathesis, *chimie douce* (polyol, co-precipitation, ion exchange), gel combustion and sol-gel synthesis, high pressure synthesis.

(b) Characterization techniques **[6 Lectures]**

***Basic concepts*:** Structure and morphology, microscopy, diffraction, interaction of radiation (x-ray, electron, and neutron) with matter

***Structural characterization by X-ray*:** X-Ray and X-ray properties, characteristics and white radiation, Production of X-ray, interaction of X-ray with electron, form factor, structure factor, Interference

***Diffraction principle and instrumentation*:** Source, sample holder, detectors; Powder XRD and single crystal XRD, synchrotron-based x-ray diffraction, small angle X-ray and neutron scattering.
Techniques based on X-ray absorption and reflection.
***Neutron and its properties*:** Neutron source and instrumentation, interaction of neutron with atoms, form factor, structure factor, neutron diffraction
***Electron and its properties*:** Electron source and instrumentation, interaction of electron with atoms, form factor, structure factor, Electron diffraction (selected area electron diffraction, convergent beam etc.)
***Data analysis*:** Indexing, structure refinement, phase identification, quantification, structural parameters calculations

***Imaging and surface characterisation*:** Optical microscope and electron microscope (SEM and TEM), high resolution images, morphology and size, shape from electron image, polarized optical microscope, XPS, SIMS.

(c) Chemical, major, trace and ultratrace analysis **[6 Lectures]**

Terminology and vocabulary of analytical chemistry, basic overview of analytical concepts, solutions and their concentrations, stoichiometry, sample dissolution techniques.
Gravimetric methods of analysis, volumetric/titrimetric analysis, redox titration & potentiometry
Introduction to separation sciences, ion exchange chromatography.
Principal & application: Ultraviolet and Visible Spectroscopy, Atomic absorption & emission spectrometry with plasma and electrical discharge sources, mass spectrometry.
Applications of voltammetry in organic and inorganic analysis.
Applications of thermo-gravimetric, differential thermal analysis, differential scanning calorimetry and thermometric titrations.
Mass spectroscopy and Hyphenated techniques: Basic principle, instrumentation, application, classification, need for hyphenation, interfacing devices and applications of GC-MS, GC-IR, LC-MS, LC-FTIR, LC-NMR, CE-MS, HPLC-MS, HPLC-NMR, LC-PDA-MS, HRMS/LC-MS-MS, LC-NMR-MS, LCPDA-NMR-MS, Solid-phase extraction (SPE), Large volume injection (LVI), GC-MS, neutron activation analysis.

(d) Functional Materials **[11 Lectures]**

***Magnetic materials*:** Magnetic moments of electron and free atom, dia-, para-, ferro-, ferri- and antiferro-magnetism, theories of para-magnetism and ordered magnetism, magnetic phenomena: hysteresis and related properties, magnetic anisotropy, magnetostriction. magnetoresistance, magnetic domains, domain theory, magnetization processes in terms of domain theory, multiferroic materials and their applications as sensors and actuators, functional materials in computer memory devices: Ferroelectric RAM, phase change materials in optical media storage devices, Giant and colossal magnetoresistance materials and their applications.

Energy materials

Batteries – primary and secondary batteries, lithium-ion battery, components and processes in batteries, cell characterization, large scale applications, energy Vs power density, different types of supercapacitors (Electrochemical double layer capacitor, pseudo capacitor and hybrid capacitor), components of supercapacitors, electrochemical properties (charging/discharging cycles, cyclic voltammetry and impedance spectroscopy, lifetime stability), concept of fuel cells.

Photovoltaics: Solar energy and energy conversion, fundamentals of semiconductor physics and photovoltaic cells, generation-recombination in semiconductors, p-n junction, metal semiconductor and hetero junction, photovoltaic device fabrication and characterization, current status of silicon based solar cells, advancement in photovoltaic research and design of new generation solar cells (hybrid, quantum dot, dye-sensitized and perovskite solar cells)

Thermoelectric materials: Fundamentals of thermoelectricity (Seebeck, Peltier and Thomson effects), thermoelectric effects and transport properties, basics of thermoelectric devices, heat conduction in bulk thermoelectric materials (heat conduction by phonons, heat conduction by electrons), progress in thermoelectric materials (bulk thermoelectric materials, nanostructured thermoelectric materials), reduction of thermal conductivities in bulk and nanostructured materials), thermoelectric devices.

Materials for heterogeneous catalysis: Renewable energy and renewable fuels, basic principles of catalysis, photocatalytic and photoelectrochemical materials for solar fuel production from water and CO_2, thermochemical hydrogen generation, catalysts for the conversion of biomass-derived feed stocks into fuel components, electrocatalysts for water electrolysis and CO_2 reduction.

Device-worthy materials***:*** Important elemental and compound semiconductors - Ge, Si, Te, II-VI, III-V, IV-VI and amorphous Si. Single crystal growth techniques – float zone – Czochralski – hydrothermal growth – growth of Si – growth of GaAs – Production of Si and GaAs. Wafers– growth of quartz. Thin film deposition techniques – thermal and electron gun evaporation –DC and RF sputtering. Epitaxial film deposition techniques – CVD, VPE, LPE and MBE, technique for 2D and 3D printing.

Suggested references

1. Solid State Chemistry and its Applications by A. R. West
2. Material Science and Engineering by V. Raghavan
3. New Directions in Solid State Chemistry by C. N. Rao and J. Gopalakrishnan
4. Solid State Chemistry: An Introduction by Smart and Moore
5. Introduction to Solid State Physics by Charles Kittel
6. Advanced Techniques for Materials Characterization" Eds. A. K. Tyagi, M. Roy, S. K. Kulshreshta, S. Banerjee, Trans Tech Publications Ltd, Switzerland (2009)
7. Advanced Inorganic Chemistry, 6th Edition by F. A. Cotton, G. Wilkinson, C. A. Murillo, M. Bochmann
8. Inorganic chemistry by Shriver & Atkins, 5th edition
9. Inorganic Chemistry: Principles of Structure and Reactivity, 4th edition, by J. E. Huheey, E. A. Keifer, R. L. Keifer, O. K. Medhi
10. Culity, Introduction to Magnetic materials, Addison Wesley (1972)
11. Linden D. and Reddy Thomas B., "Handbook of Batteries", 2001, McGraw Hill Publications
12. Functional Materials: Preparation, Processing and Applications, S. Banerjee (Editor), A. K. Tyagi (Editor) (2011)
13. Thermoelectrics: Basic Principles and New Materials Developments, G.S. Nolas, J. Sharp, J. Goldsmid (2001)
14. Heterogeneous Catalysis for Energy Applications Editors: Tomas R Reina, Jose A Odriozola, Energy and Environment Series No-27, The Royal Society of Chemistry, Printed in the United Kingdom by CPI Group (UK) Ltd, Croydon, CR0 4YY, UK, Publication date: 11 Sep 2020, Print ISBN: 978-1-78801-718-3
15. J. R. H. Ross, Contemporary Catalysis, Fundamentals and Current Applications, 1st Edition, Elsevier, 2018.
16. Photocatalysis Science and Technology, M. Kaneko, and I. Okura (Eds.), Springer, ISBN 3-540-43473-9.