Summary Report

About Department/Center/School: Materials Science Centre at IIT, Kharagpur, the first one of its kind in the country, was founded in 1970, in order to promote interdisciplinary research and education. The main research of the Centre focuses on semiconductor, polymer, and ceramic materials including nanomaterials. After an M.Tech. program started in 1980, the Centre is providing education on the above disciplines of Materials Science. The research areas have been evolving to new materials such as carbon nanotubes and graphene, and device technologies. Currently, the main active research areas of the Centre are energy materials (for batteries, fuel cells, solar cells and thermoelectrics), magnetic materials, and polymer membranes and nanocomposites.

1. Academic Programs (Range of Degrees and Disciplines):

- *i) M.Tech in Materials Science and Engineering 2 years' duration*
- ii) M.Tech+Ph.D in Materials Science and Engineering 2 years' MTech followed by an optional enrolment in the Ph.D programme, provided fulfilled required criteria
- iii) Ph.D
- 2. **Major 4-5 Thrust Areas of Research**: i) Semiconducting Materials; ii) Multiferroic materials; iii) Polymer membranes and composites; iv) Supercapacitors and Li-ion batteries, v) Fuel Cell and Catalysis.

3. Curriculum and Courses & Teaching Environment

Items	Ratio/	Items	Number/%
	Number		
Teacher-student Ratio	1:12	Average No. of students motivated (%) to opt of careers Eng/ Tech. Sectors UG/PG/PhD	NA/30/10
No. of Faculty members as on today	10	Average No. of students motivated (%) to opt of careers in Science sectors UG/PG/PhD	NA/70/90
Average No. of Tutorial Assistants	20	No. of teaching labs	4
No. of UG/DD students	NA	Average No. of students per experiments in core courses	4
No. of PG students/PhD students	58/66	No. of Students' workshops/`Tinkering'' Labs	0
Average no. of tutors with more than 100 students	0	No. of new courses introduced	01
Average Students placements (%) (UG/DD/PG)	NA/NA/<50	No. of New program introduced	0
No of major curriculum review in both UG & PG level	1	Undergraduate vs PhD strength expressed as Percentage	NA
No of UG lab (teaching labs) developed/set-ups	NA	No of PG/research labs developed/new set up	2
No of E class rooms	2	No. of lab classes per week	1
Average No. of Course done per	NA/NA/16/4	No. of core/elective/seminar/projects	NA

student for B. Tech/DD/M.	subjects taken for B. Tech, DD, and M.	NA
Tech/Ph.D	Tech respectively	06/05/02/02

4. Research and Development & its Environment

Items	Number	Items	Number	Items	No.
Total No. of Publications in Journals (2008-13)	524	Average no. of citation per paper	5.43	No of large interdisciplinary research projects	0
Total No. of Publications in Conference & Symposium	NA	Average Journal publication per year	105	Number of Int. conf./workshops attended by students	60
Total No of Books & e-books published	0	h-Index of the department since 2008/overall h-index in Scopus	20/165	No. of PDF hired in the Institute	0
Total No of Edited Conference Proceedings/book chapters	0/9	Number of papers with citation more that the average no. of citation of the Journals	60	No. of international Students as PhDs/PDFs	0
Total No. of Technology Developed/transferred	0/0	No. of recognitions & Awards, fellows etc to faculty/students (provide break up if necessary)	11/NA	No. of International visiting researchers/adjunct faculty stayed here for at least a week	05/00
Total No. of Patents Filed/Obtained	13/04	Average Retention(%) of Young faculty for at least 10 years	70	No. of short courses / workshops /conf. organized with international participations	00/00/00
Total No. of Copyright Filed/Obtained	0/0	No. of Sponsored research Project /fund(lakh) generated from non-internal source	50/600	Average No. of PhD granted per year	12
No. of Publications per Faculty/Masters/PhD students	50/01/04	No. of Consultancy /fund (lakh) generated from non-internal source	07/31	Average No. of PhD Granted per year per faculty	01
No. of Publications per Faculty/Masters/PhD students in Top Ten Journals as Identified by the department	10/00/02	No of Internal and external Collaborations research papers /research projects/PhD students	60/3/0	Patent granted per faculty	0.4
Average No. of Citation per faculty per year	55.32	No of M. Tech students motivated into pursuing	62/46	Number of articles in collaborations with Ten countries*	50

		PhD/PhD graduates motivated to pursue career in Academics (abroad or IIT etc)			
Ranking of the department in terms of average citations per paper within the Institute	7	Ranking of the department in terms of total number of Journal publications within the Institute/publications per faculty	11	No of articles of the dept. contributing towards h-index of the Institute since 2008	10

5. External Stakeholder Engagement and others

Items	Number	Amount Lakh
No. of PhD/Master students' thesis funded by Industries	0/0	NA
Total number of Industry sponsored projects and its income (Lakh)	02	55
No. of Curriculum Development Initiative for Industries	NA	NA
No of Technology transfer/adopted by Industry/Labs	0/0	NA
No. of Nationally relevant research projects	0	NA
No of Policy inputs/consultancies provided	06	NA
No. of Research grant and seed money from internal savings of the 02 30		30
Institute per young faculty of the department and its total fund	02	30
No. of Community Relevant projects	0	NA

6. Vision for the Future (in brief):

(a) Departments/centers/schools should spell out its Mission and Vision Statements, (b) Plans for future to achieve the projected goals and (c) measures adopted towards above.

Our Centre primarily focused on the interdisciplinary research areas such as polymer, ceramic and semiconducting materials. Keeping in mind on the energy crisis/demand and global warming, our faculty members are engaged and would continue in the research and development of following research fields/areas. In particular, our Centre research would emphasize on the synthesis, characterization and applications of advanced materials for the next generation.

- (a) Energy materials. This includes materials for fuel cells, Li-ion batteries, supercapacitors, solar cells and thermoelectrics.
- (b) Hybrid materials including polymer nanocomposites, polymeric membranes, polymers for gas sensors and separation, and ceramic materials for gas sensors.
- (c) Magnetic materials such as multiferroic thin films, nanofluids and composites.

7. External peer review of the Dept./centre/schools (in brief): (a) Date: May, 2013

(b) Name of the Experts involved and their affiliations in short: (1). Prof. Arup K. Raychaudhuri, Director & Distinguished Professor, S. N. Bose National Centre, Kolkata, (2) Dr. A. K. Saxena, Director, Defense Materials Stores, Research & Development Establishment (DMSRDE), Kanpur, and (3) Dr. A. K. Tyagi, Head, Materials Science Division, Bhaba Atomic Research Centre, Mumbai

(c) Overall recommendations of the peer review committee: Strengths, weaknesses, suggestions and comments

The Centre is doing well above the expectation on the sponsored research, journal publications, and short courses, and performing well on the teachings, availability of teaching/research lab facilities. However, improvement is suggested on identifying fewer areas and thus making an impact. Furthermore, following suggestions were provided by review committee members for improvements.

- Departmental library should be made available to M.Tech. students
- The downtime of major facilities should be minimized. A better mechanism should be in place so PhD students can get more access to central facilities i.e. FESEM, HRTEM and XPS
- There should be enhanced interaction between PhD students and faculty members
- There should be provision of sending PhD students abroad to attend international conference
- Interaction of M.Tech. and PhD students with industries.
- The laboratory safety manual should be made available to all the students. Safety gears (goggles, gloves etc.) should be made available to students.
- A computational facility at the Center would be added benefit for research.

(d) Measures adopted/action taken at the department level to address the recommendations of the peer review report:

Our Centre has identified a few areas to focus on for next few years to make an impact that has in accord to the requirement of Vision 2020. In particular, our Centre is aggressively upgrading lab facilities to international standard. Although we have been publishing large number papers in the reputed international journal, focuses is given to quality research and publish at least 30-50% of paper in the top 10 journals indentified by the Centre.

8. Strengths, Weaknesses, Opportunities & Threats (SWOT) Analysis of the Department

STRENGTHS

√ Number of PhD students, advance research and int. journal publication output

 $\sqrt{\text{Interdisciplinary research and teaching}}$

√ Good quality faculty

√ Only a few such Centre/departments (2-

- 3) in our country, First of this Centre in the country
- √ Conferences and continuing education programmes organized on regular basis √ Periodic feedback of the students

WEAKNESSES

√ Maintaining the existing research infrastructures

√ Low teacher-staff especially technical staff ratio

 $\sqrt{\text{Low national and international awards}}$

 $\sqrt{}$ Inadequate linkages with industry and community

OPPORTUNITIES

- √ Can contribute significantly to energy and environment issues, and polymeric materials (this is one of the unique discipline of this Centre in our country)
- √ Acquire more number of patents and perform towards technology transfer
- $\sqrt{}$ Possibility of more international and national collaborations and joint ventures
- $\sqrt{\text{Training of technical supporting staff}}$
- √ Developing labs, chair professorships, collaborative programs with world class universities/ industries of international repute.

THREATS

- $\sqrt{}$ More attractive opportunities outside the IITs pose greatest threat to attract and retain good quality faculty and technical staff
- $\sqrt{}$ Immediate requirement of faculty is needed as several senior faculty members are to retire in next 2-3 years.
- √ Lack of incentives for quality research

*Note: Ten countries: US, UK, Germany, Japan, Canada, France, Italy, Australia, Singapore, South Korea

Important Highlights

Materials science centre is engaged in the following research and development activities:

- 1. Nanostructured materials for energy, photonic and sensor application
- 2. Novel materials for membrane based separation, proton exchange membranes, batteries and thermoelectric application
- 3. Polymeric blends and composited for super-capacitor and EMI shielding.

Development materials for Li-ion batterie

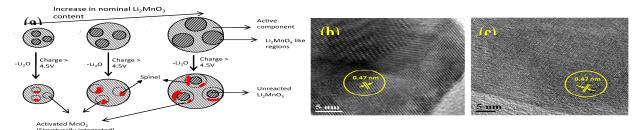
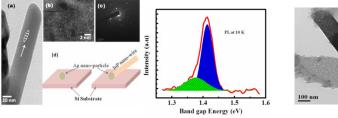
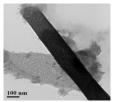


Figure 1 (a) Schematic model on the development of electrochemically triggered spinel phase in Li₂MnO₃-LiMn_{0.375}Ni_{0.375}Co_{0.25}O₂ composite cathodes. (b) and (c) show the HRTEM image of the virgin and cycled cathode. Details available in C. Ghanty, R.N. Basu, and S.B. Majumder, Electrochimica Acta (2014) (in press) http://dx.doi.org/10.1016/j.electacta.2014.03.174

Siver nanoparticle assisted MOCVD growth of InP nanowires on (100) p-Si substrates. TEM image of a single nano-wire at (a) low magnification (b) high magnification. SAED pattern showing single crystalline nature of the nano-wires. (d) Schematic of the mechanism of VSS growth of InP NWs. Photo luminescence spectra of the NW ensemble taken at 10 K. The convoluted peaks suggest recombination due to band to band and excited states. TEM image of InGaAs nanowires grown on (100) p-Si substrate by MOCVD technique and its SAED pattern [Appl. Phys. Letters 101, 212108 (2012); J. Appl. Phys. 115, 043101 (2014)].

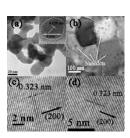


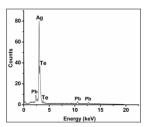


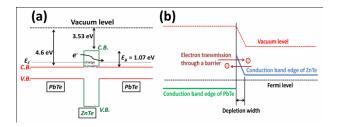


A typical TEM image of PbTe:Ag nanocomposites showing the formation of densely packed grains with embedded Ag-rich nanodots. The introduction of the appropriate energy barriers at the grain interfaces and the inclusion of Ag-rich quantum dots within the grains of the PbTe:Ag nanocomposite samples are found to be the key factors to control the energy dependency of scattering of the carriers, i.e. energy filtering of the carriers. A remarkable enhancement of Seebeck coefficient of the nanocomposite samples by the energy filtering of the carriers in the temperature range 300 - 600 K is achieved. The reduced lattice thermal conductivity in PbTe by ZnTe nanostructures leads to notable enhancement in figure of

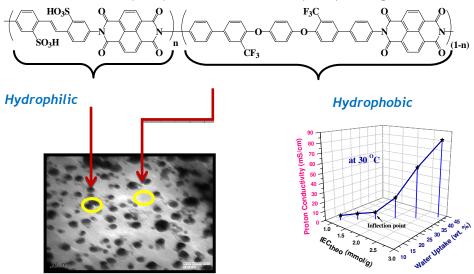
merit with a maximum value of 1.35 at 650 K [J. Appl. Phys. 108, 064322 (2010), ACS Applied Materials & Interfaces (DOI: 10.1021/am405410e)].



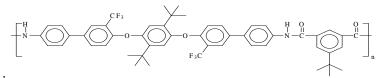




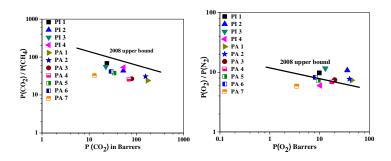
Development of new polymers for proton exchange membrane fuel cells (PEMFCs) have become a very active research area for both mobile and stationary applications. Compared to other energy converting devices, PEMFCs are eco-friendly with higher energy efficiency. New protonexchange membrane (PEM) materials with good properties are the most important and challenging parts in this research field. Material Science Centre of IIT Kharagpur is also engaged in the developments of new high performance PEM materials for fuel cell application. In this context, researchers are working on different kind of advanced sulfonated high performance polymers like poly (aryleneether)s (PAE)[1,2], poly(ether imide)s [3,4] etc. During last 3-4 years they have developed different series of semifluorinated sulfonated copolymers with controlled degree of sulfonation. The polymers are easily processable with high molecular weight and gave tough, flexible and transparent membranes. Oxidative and dimensional stability of the membranes was improved by introducing trifluoromethyl substituents in the copolymer structure. The copolymer membranes showed significantly high proton conductivity(up to 136 mS.cm⁻¹)with low activation energy which are in the range of commercially available Nafion® membrane. In addition to this the synthesized polymers exhibited high thermal stability ($T_g \sim 220$ °C, $T_{d5} \sim$ 300°C)and superior mechanical property(tensile strength up to ~105 MPa, elongation at break ~ 36%) higher than many other aromatic sulfonated polymers. Microscopic analyses by TEM revealed well-dispersed hydrophilic domains (following figures) that contributed to better proton conducting properties [Industrial & Engineering Chemistry Research, 52(2013) 2772, Journal of Membrane Science, 441 (2013)168, RSC Advances, 4 (2014) 11848].



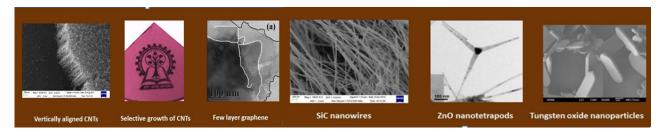
Membrane-based gas separation has established as a superior, economical and efficient separation technique over other conventional methods. Polymer membranes find various attractive applications such as removal of carbon dioxide from natural gas for fuel efficiency and to reduce the pipeline corrosion by CO_2 contaminant in the natural gas. In our Materials Science Center we are engaged in developing different types high performance processable polymers such as polyimides, polyamides etc. for membrane-based gas separation application. The polymer membranes developed by us showed a good combination of permeability and selectivity for different gas pairs. They are close or some time surpass the 2008 Robeson upper bound as shown in the following figures (which has been drawn by Robeson to set the standard for the gas permeable membrane). In addition to their gas separation efficiency these membrane showed superior thermal ($T_g \sim 270$ °C, $T_{d10} \sim 400$ °C) and mechanical property (tensile strengths ~ 90 MPa, elongation at break $\sim 15\%$) which are prerequisite for the membranes applied in gas separation application [*Journal of Membrane Science 365 (2010) 329, Journal of Membrane Science447 (2013) 413*].



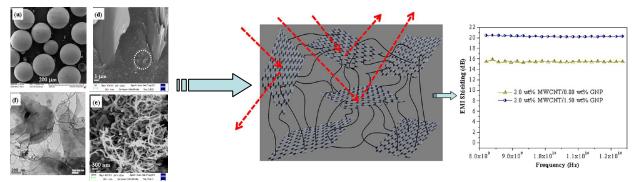
PA 1()with best combination of permeability selectivity



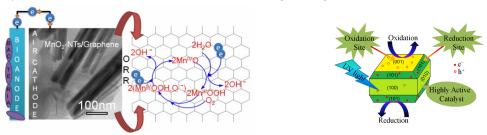
The design and fabrication of an MOCVD reactor for Silicon Carbide epitaxial films was done for the first time in the country. The reactor was used to grow low defect density epilayers of SiC on Si as well as to fabricate SiC nanowires and nanopowders. A CVD reactor was again fabricated and used to understand basic growth mechanisms of CNTs. It was clearly demonstrated that the VLS mechanism is inadequate to explain growth of CNTs in many cases. Catalyst-free growth of CNTs was also demonstrated. Growth of different types of nano-structured materials have been undertaken, such as CNTs, Graphne, Sic, ZnO, etc [Nanotechnology 21(2010) 415605; Carbon 48 (2010) 2371]



In-situ polymerization of styrene/multi-walled carbon nanotubes (MWCNTs) in the presence of suspension polymerized polystyrene (PS)/graphite nanoplate (GNP) micro-beads, for the preparation of electrically conducting PS/MWCNT/GNP nanocomposites with very high (~20.2 dB) EMI shielding value at extremely low loading of MWCNTs (~2 wt %) and GNP (~1.5 wt %) is demonstrated. Finally, through optimizing the ratio of PS–GNP bead and MWCNTs in the nanocomposites, an electrical conductivity of $\Box 9.47 \times 10^{-3}$ S cm⁻¹ was achieved at GNP and MWCNTs loading of 0.29 and 0.3 wt %, respectively. The random distribution of the GNPs and MWCNTs with GNP–GNP interconnection through MWCNT in the PS matrix was the key factor in achieving high electrical conductivity and very high EMI shielding value at this low MWCNT and GNP loadings in PS/MWCNT/GNP nanocomposites. With this technique, the formation of continuous conductive network structure of CNT–GNP–CNT and the development of spatial arrangement for strong π – π interaction among the electron rich phenyl rings of PS, GNP, and MWCNT could be possible throughout the matrix phase in the nanocomposite [*ACS Applied Materials and Interfaces*, 5, 4712-4724 (2013)]



MnO₂-NTs/graphene composite is demonstrated as promising cathode catalyst to replace expensive platinum in the microbial fuel cell for power generation and wastewater treatment. [S. Khilari, S. Pandit, M. M. Ghangrekar, D. Das, D. Pradhan,* *RSC Advances* **2013**, 3, 7902-7911.]. Synergy of Low-Energy {101} and High-Energy {001} TiO₂ Crystal Facets for Enhanced Photocatalysis [*ACS Nano* **2013**, 7, 2532–2540] – this figure is given to SNST



During the past two decades, a large variety of nanostructured materials of metals, alloys, intermetallics, ceramics, composites, and cermets. We developed and explored several chemical methods, which allowed tailoring specific morphologies of nanoparticles in strictly controlled manners, with useful functional properties for electronics, magnetics, magnetoelectronics, photonics, structures, biological and gas sensors, solid fuels, and related devices. We prepare the materials in the forms of nanofluids, films, discs, and other engineering shapes. The research approach unites interests and expertise from development of novel functional materials and their science & technology, and studies and simulation/modeling of microstructures and thermal, magnetic, structural, and other properties, and stability and phase transformations. Major research projects carried out can be briefed as follows: The magnetic as well as nonmagnetic powders consist of controlled crystallite size of 20 to 100 nm. Metal oxides are in 5 to 20 nm quantum confined size. Mesoporous Al₂O₃ ceramic composites are available in amorphous as well as in selective polymorphic forms. Crystalline powders consist of 5 to 20 nm particles/crystallites separated through 2 to 5 nm pores. In-situ synthesis of nanogold dispersed in an optical host; (A) Al₂O₃ (powder) and (B) polymer (nanofluids & films) [International Nano Letters, 3 (2013)17; Journal of Nanofluids, 2 (2013) 249]

