MANIPAL UNIVERSITY
JAIPUR

Report on
Collaborative visit in Flinders University, Adelaide Australia

April 9 - 23, 2017

Dr. Pushpendra Kumar

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Report

Visit to Flinders University, Adelaide, Australia

1. Name, Designation with department	**Dr. Pushpendra Kumar** Associate Professor Department of Physics, Manipal University Jaipur Jaipur-303007, Rajasthan, India
2. Host Faculty and Department(s)	**Prof. Gunther Andersson** Professor of Chemical Physics and Nanotechnology Research Leader Flinders Centre for NanoScale Science and Technology School of Chemical and Physical Sciences Flinders University, GPO Box 2100, Adelaide SA 5001, Australia Email: gunther.andersson@flinders.edu.au
3. Date of visit	April 9-23, 2017
4. Invited Talk **Date:**	**Title: Functionalised Porous Silicon for Energy Storage Applications** **Short Abstract:** Nano-porous materials are a subset of nanostructured materials and possess unique properties for various applications. The porous silicon (PS) has been a material of great interest because of its easy synthesis by electrochemical methods and better control on physical properties e.g. porosity, length and pore diameter. PS has been used to study several fundamental phenomena and has large number of technical applications in LED, sensors, separation, hydrogen generation, catalysis, biological molecular isolation and supercapacitor for energy storage. Photoluminescence (PL) appearance in porous silicon (PS) has attracted a large scale investigations. The PL study in PS with decreasing Si crystallites size among the pores was studied. The PL appearance is attributed to electronic confinement in columnar-like (or dotlike) structures of porous silicon. Different pore diameter PS samples were prepared by electrochemical etching in HF-based solutions. Changes in porous silicon and Si crystallite size were studied by using Brunnauer-Emmer-Teller model (BET), Raman scattering, Fourier transform infrared spectroscopy (FTIR), scanning electron microscope and electron transmission spectroscopy. Further, the porous silicon was used as template to confine the organic and inorganic materials in the nanopores of PS to study the confinement effect on its optical, structural and magnetic properties. In addition to that, PS coated with ultrathin graphene layer is being used as electrode materials for the promising new platform for grid-scale and integrated electrochemical energy storage applications. **April 18, 2017**
5. Seminar Attended	Annexure I
6. Laboratory and research facility visited (with Photo)	Annexure II
7. Other Faculty members and researcher you interact	Prof. Joseph Shapter Prof. Sarah Harmer-Bassell Prof. David Lewis Prof Claire Lenehan Dr Chris Gibbson Dr Anirudh Sharma Prof Chris Franco

	Yanting Yin Jesse Daughtry
8. Collaborative Discussion Output	Annexure - III
Any other Lab/University visited during the period	
9. Name(s) with Affilation	**Prof. Greg Metha, University of Adelaide**
10. Reason(s)	Collaborative discussion, Lab visit and Invited Talk
11. email address(es)	greg.metha@adelaide.edu.au
12. Other researcher and student you interacted	Dr. Jason Alvino, University of Adelaide Mr. Aidan Karayilan, University of Adelaide
13. Outcome from the visit	Annexure IV

Pushpendra Kumar,

Name and Signature of Visiting Professor

Annexure I

Honors seminar, Flinders Centre for Nanoscale Science and Technology

On April 10-11, 2017 (9:30 hrs to 12:45 hrs) I attended honors seminar by master students of Flinders Centre for NanoScale Science and Technology. In the honors presentation the master students presented their research project work progress in front of panel members and common audience. This is an interactive sessions and suggestions are given by the experts to the students. The following presentations are delivered by the students:

Title1: Provenancing of raw and roasted coffee beans by Peter Tram
Title2: Polysulfide polymer for capturing pollution and recovering valuable metal by Salah Alboaiji
Title3: Sulfur polymer as slow release fertilizers by Firas Andari
Title4: Improving a method for making pure birnessite by Faisel Bin Hudayab

Interaction with Professor David N. Jamieson

Special lecture by **Professor David N. Jamieson**, Ion Beam Program Manager, Centre for Quantum Computer Technology, The University of Melbourne
Venue: University of Adelaide
Date: 11th April 2017
Time: 18hr to 19hr
Talk Title: Power, Energy and health

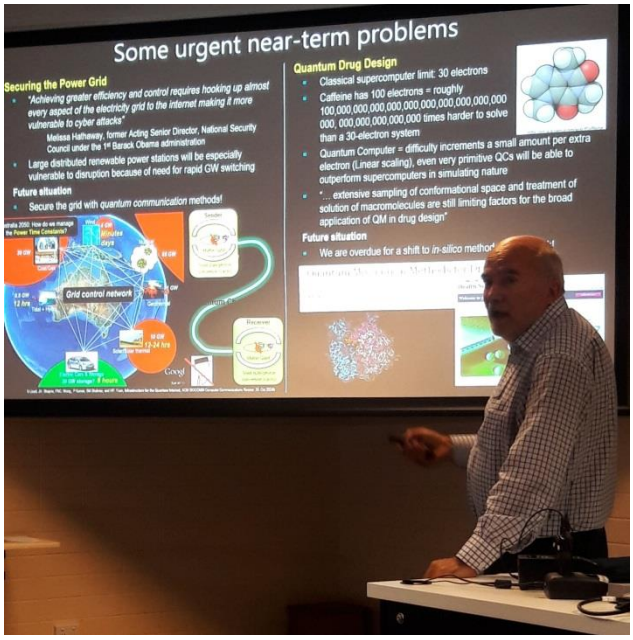


Photo 1. Presentation by Professor David N. Jamieson on energy and power.

Invited lecture by Professor David N. Jamieson, Ion Beam Program Manager, Centre for Quantum Computer Technology, The University of Melbourne
Venue: Flinders University, Adelaide
Date: 12th April 2017

Time: 13 hrs to 14hrs

Talk Title: Quantum computer devices built from implanted single atoms

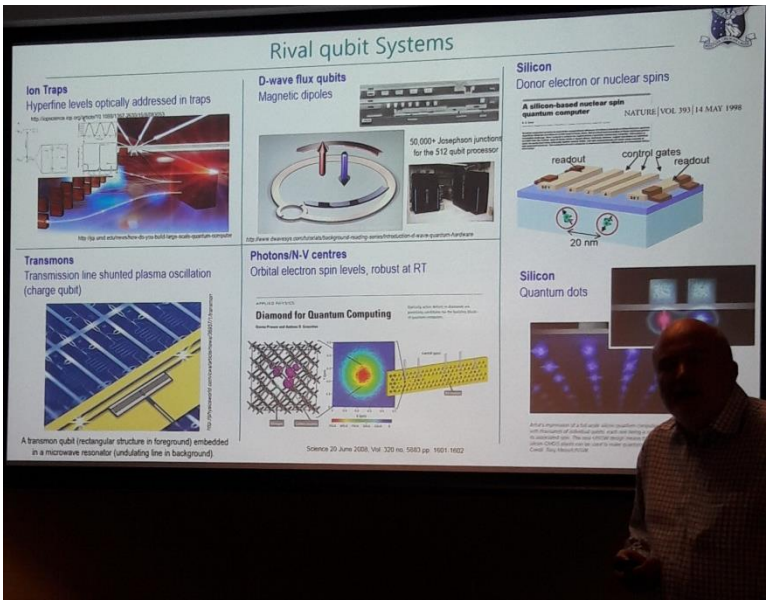


Photo 2. Presentation by Professor David N. Jamieson on single electron transistor and quantum computation.

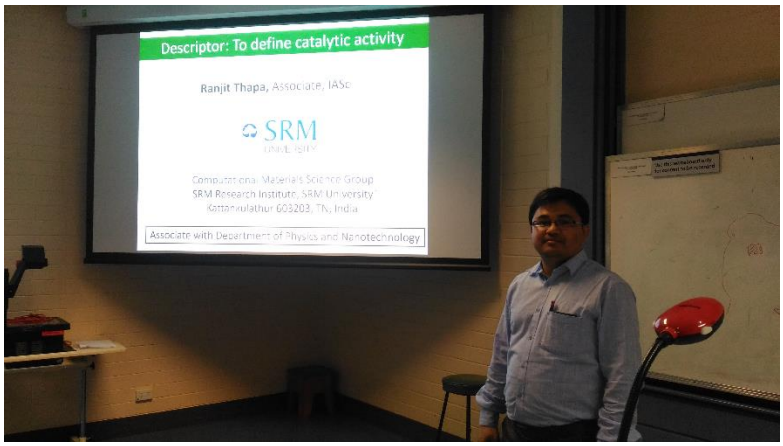


Photo 3. Presentation by Dr. Ranjit Thapa, SRM University, India on the title: Descriptor: **To define catalytic activity**

Meeting with the researcher from Flinders University, SRM University and University of Adelaide, about the future collaboration and project.

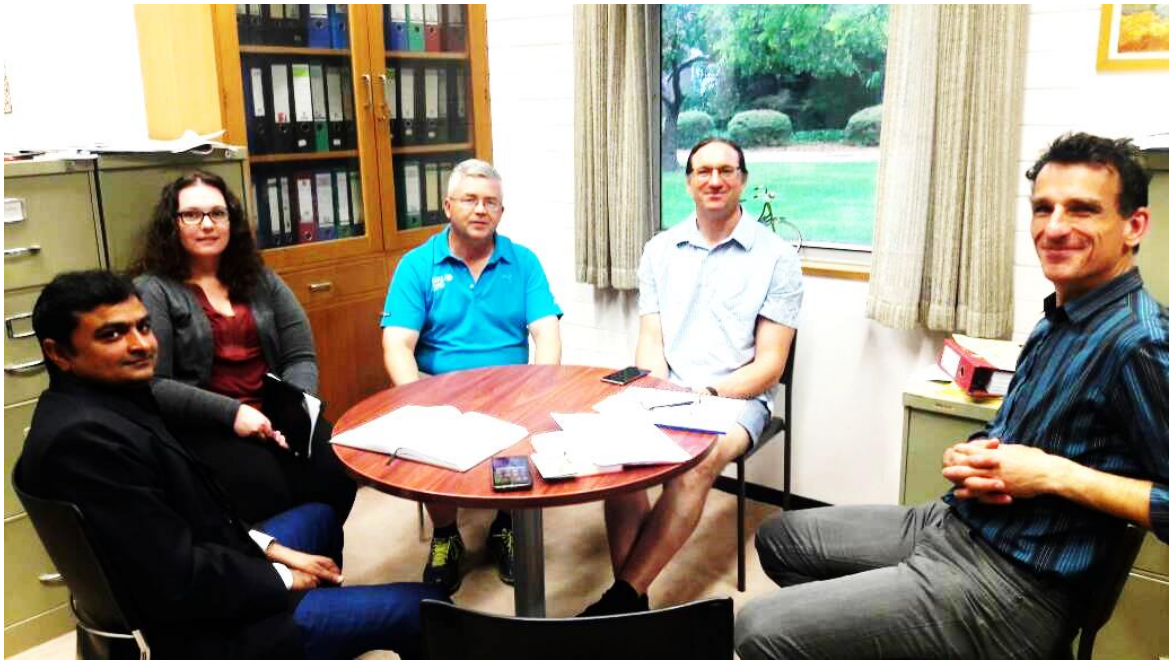


Photo 4: In this photo from left, Dr. Pushpendra Kumar, Prof. Sarah, Prof. Joseph, Prof. Greg and Prof. Gunther during the discussion meeting on 20th April 2017.

Following points are discussed during meeting.

- Start short collaborative projects, one in ferrite batteries and one in photovoltaic, suitable for 6 month projects for exchange students
- Use nanoporous materials
  - Do particles move easily into the nanopores?
  - Would a porous membrane with flow through be better suited?
  - Use STXM/TEM EChemcell for identifying crystal structure of nanoparticles in pores
- Photocatalysis
  - Nanoporous Si has an increased bandgap of 2.5 (compared to 1.3 for pure Si) due to an increas in the conduction band position, which makes it suitable for photocatalytic water splitting or CO2 reduction
  - ZnO and TiO2 can be used for nanoporous materials as well.
  - Develop descriptor for photocatalysis from DFT calculations?
  - Decide on material for nanoparticles for photocatalysis, potentially based on the choice of the descriptor derived from the DFT calculation
- Ferrite batteries
  - Largest challenge will be making ferrite nanoparticles
  - Grow ferrite nanoparticles on graphene or SiO_2
  - In situ spectroscopic analysis of ferrite nanoparticle growth using Echem cell for TEM

Discussion with Professor David Lewis, Director, Flinders Nanotechnology on 20th April 2017. He explained about the structure of Flinders University and elaborately describe about the research activity at Flinders Centre for NanoScale Science and Technology. More important points discussed are highlighted in Annexure III.

Annexure II

Facility visited at Flinders University

Electron Spectrometer for surface analysis by X-ray photoelectron spectrometry (XPS) and Auger Spectroscopy (AES)

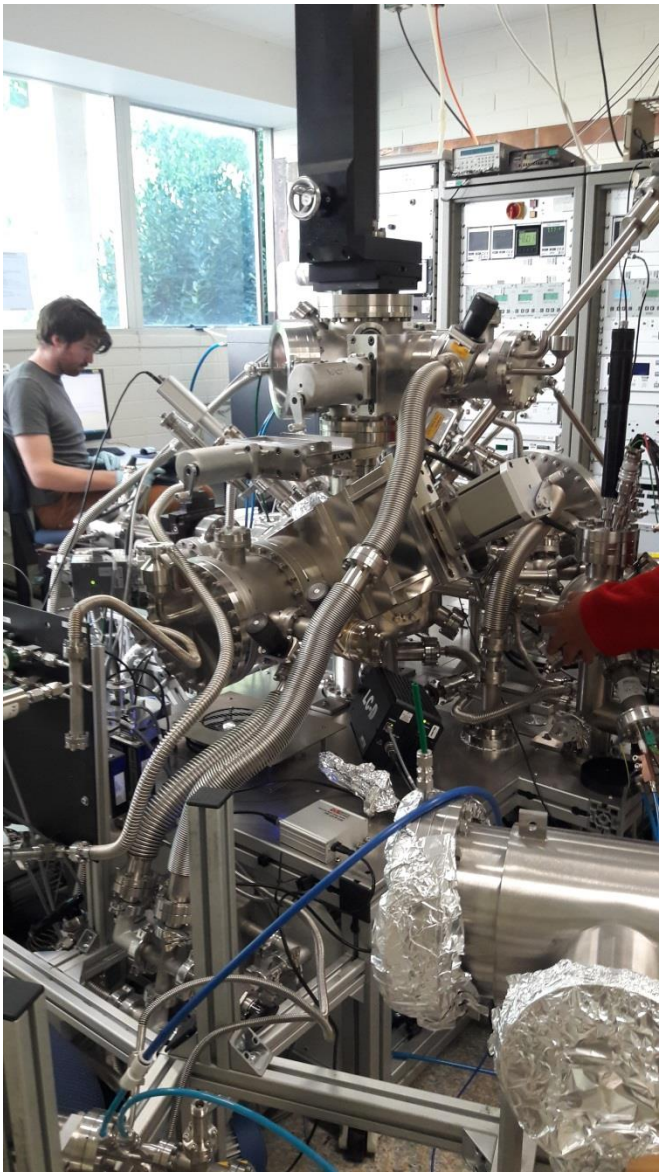


Photo 5: Metastable Induced Electron Spectroscopy (MIES) system enables measurement of the composition and electronic structure of the outermost layer of a surface. This is complemented by Neutral Impact Collision Ion Scattering Spectroscopy (NICISS) which measures concentration depth profiles with sub-nm depth resolution. These are the only systems of their kind in Australia.

Photo 6. Horiba XploRA Raman and tip enhanced Raman spectrometer

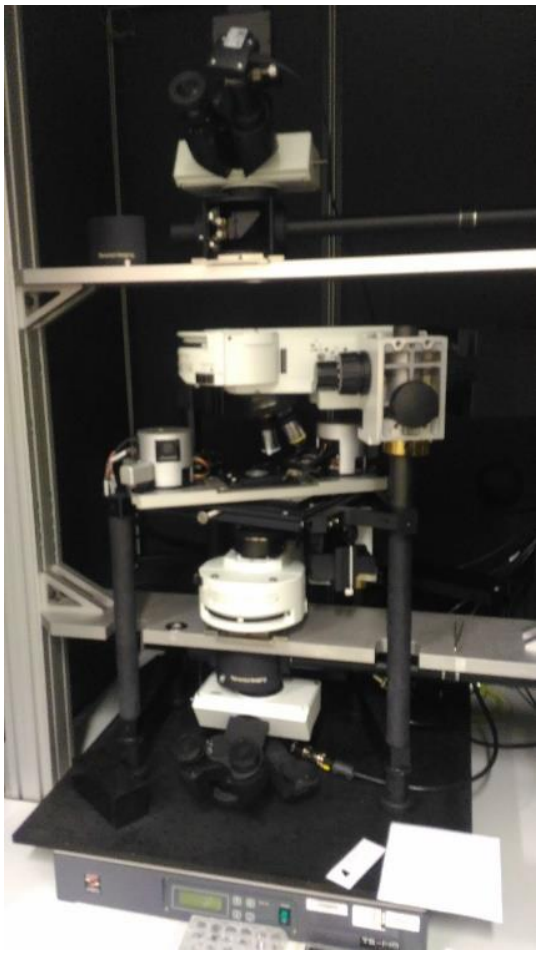


Photo 7. Tip enhanced Raman spectroscopy is used to enhance the signal intensity that works based on resonance frequency of tip and the surface of the samples. The technique is equipped with three different lasers of wavelength 532 nm, 638 nm and 786 nm and a high quality CCD camera to image and focus the sample.

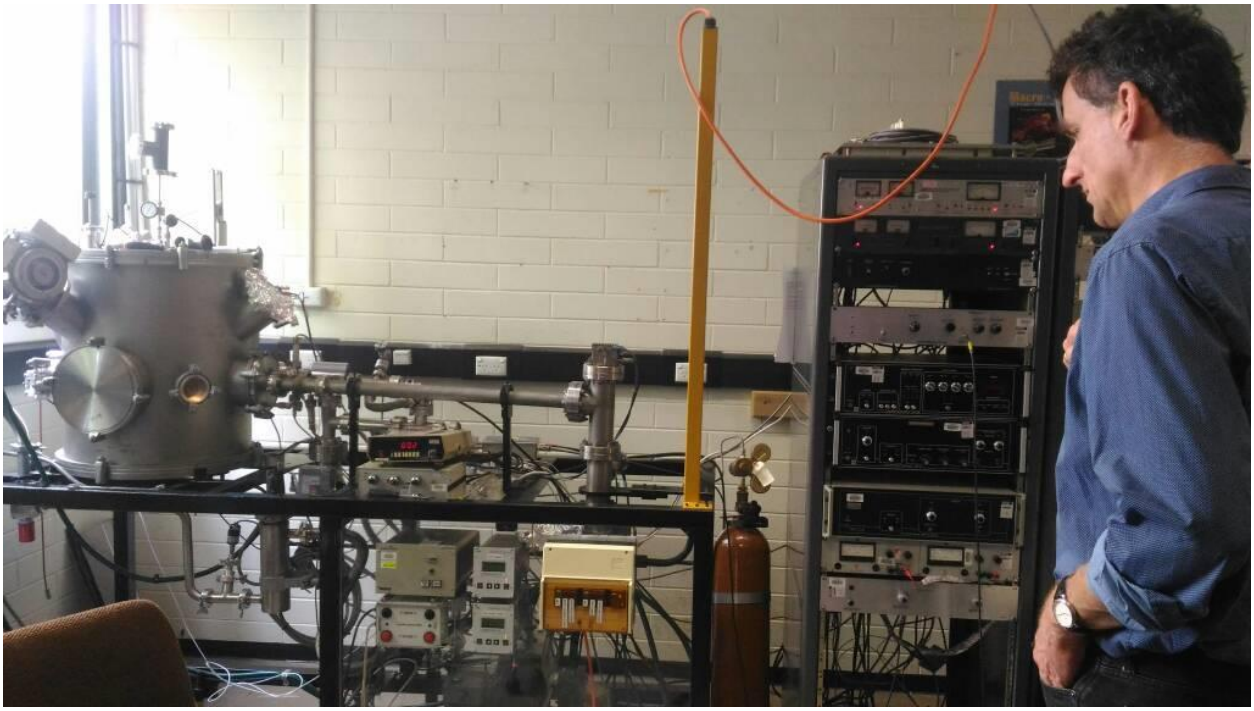


Photo 8: Neutral Impact Collision Ion Scattering Spectroscopy (NICISS) which measures concentration depth profiles with sub-nm depth resolution.

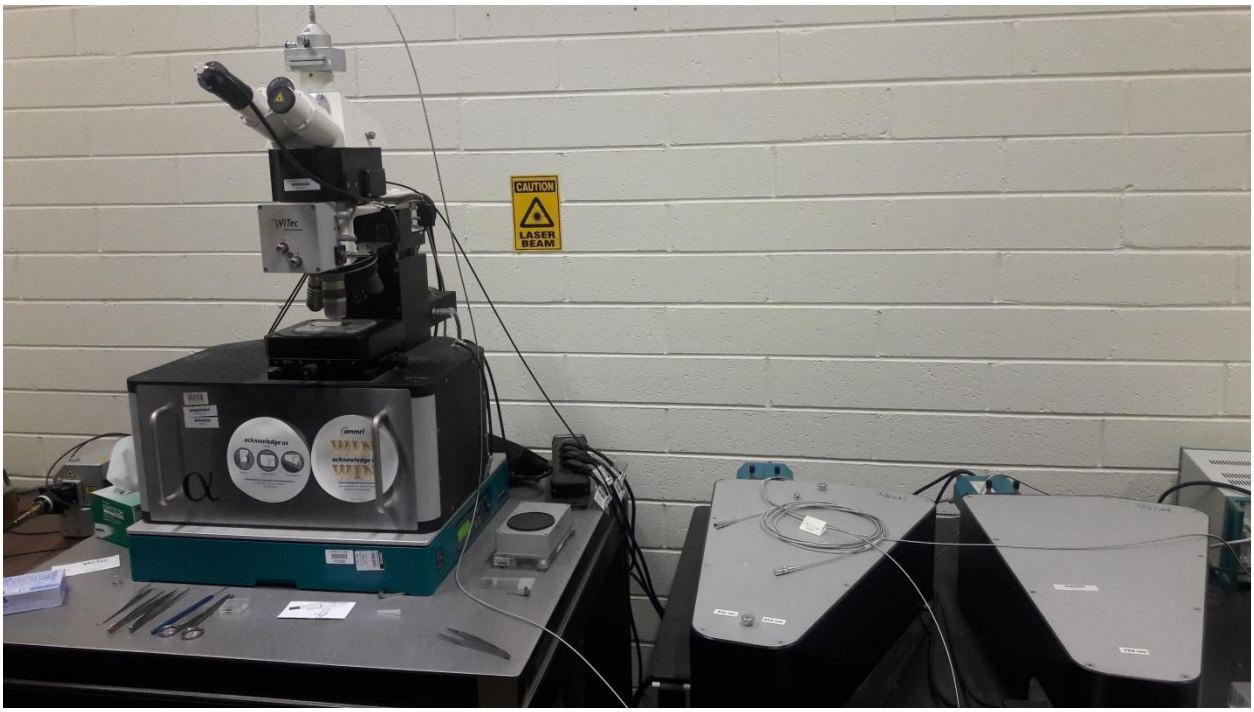


Photo 9. Raman spectrometer II (Table Top)

Photo 10. Scanning Electron Microscopy – SEM CamScan MX2500 and FEI Phenom

The CamScan instrument is a research-grade analytical SEM capable of reaching 100,000 x magnifications. High-resolution images of biological samples, metal surfaces, particles, fibres and material surfaces can be achieved with this instrument. This system also has EDX capabilities (above Z=11), whereby elemental analysis or chemical characterization of a surface can be performed. The Phenomena is a high-throughput benchtop SEM (typically 20-24,000x magnification) which allows simple and rapid analysis of samples. This instrument uses low kV backscattered detection and is capable of imaging non-conductive samples without a metallic coating.

Photo 11. Two number Novascan ESPM 3D Atomic Force Microscope and Optical Tweezer

This atomic force microscope from Novascan is mounted on a motorised inverted fluorescence microscope from Olympus (IX81). The atomic force microscope system includes both open- and closed-loop scanners, a nanolithography mode and a variety of imaging modes. The maximum scan range is 120µm by 120µm in lateral dimensions and 8 µm in vertical dimensions. This atomic force microscope is particularly suited for high sensitivity force measurements.

Photo 12. Electron Spin resonance
Electron spin resonance spectroscopy is used to study the material with unpaired electron.

Photo 13. Nano ink for lithography pattern

With this technique a nano-size pattern can be created and the created pattern further can be used to create nanostructured material and in electronic circuit devices.

Facility to develop Solar cell

Photo 14. Polymer solar cell Printer

Photo 15. Glove box to make polymer solar cell and perovskite solar cell devices under desired atmosphere.

Photo 16. Dynamic Mechanical analyzer helps to understand the mechanical properties of polymers

Annexure III

Outcome of Discussion

During our visit to Flinders University 9-23rd April 2017, numbers of meetings were held with research collaborator from Flinders University, University of Adelaide and SRM University Chennai. The concluding remarks of these meetings are as follows:

1. With reference to the outcome of our joint proposal submitted in AISRF 2016, it has been decided that few joint publication is required to make our applications more strong in bilateral research scheme.

2. The joint supervision of a Ph.D. student is the best way to strength our research collaboration and for that dual degree program for Ph.D. students is required in which one year in Flinders University and two year in Manipal University. More discussion is required to further proceed to have a joint Ph.D. student.

3. The prepared AISRF research proposal will now be submitted in other funding scheme in India by Dr. Pushpendra kumar, Manipal University and Dr. Ranjit Thapa, SRM University. Researcher form Flinders University will be mentioned as foreign Co-Investigator in the project proposal. The accommodation, local transport and living cost of two foreign researchers (faculty/student) during the visit to India for one month for collaborative work can be considered in each project proposal budget.

4. The students from Manipal University can go under internship program at Flinders University and they can work on the joint projects on mutual interest of topics. The supervisor will be from both the university to guide the students.

5. Flinders university, University of Adelaide, Manipal University Jaipur and SRM University will work together for joint publications and product.

6. The researcher from Manipal University can collaborate and use the facility of Flinders university and University of Adelaide and SRM University Chennai, vice-versa.

7. In future the joint proposal will be submitted with more precise objective and proof of concept.

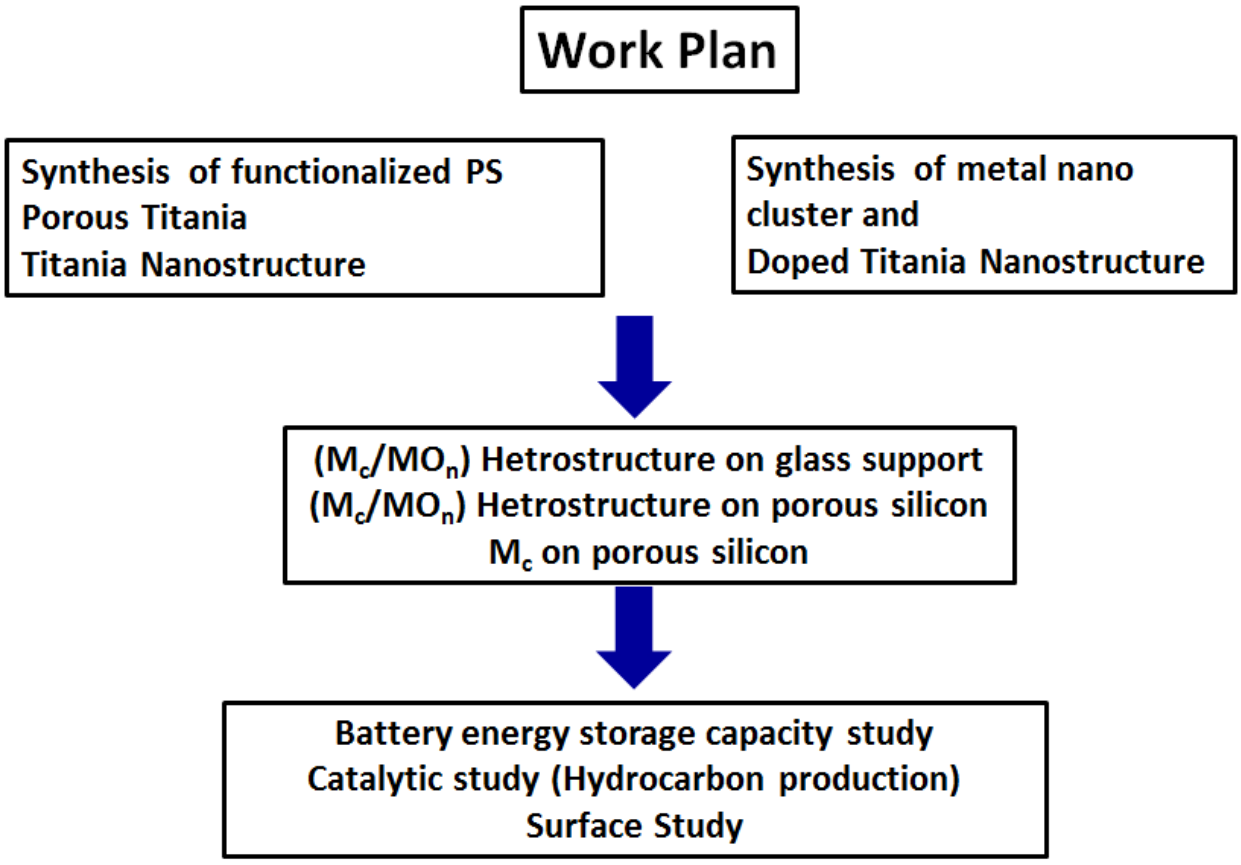
Proposed research work on Ferrite Batteries

A new approach to enhance the energy storage capacity of batteries based on porous silicon membrane functionalized with ferrate nanoparticles has been planned. The ferrate nanoparticles have not yet been used for battery electrode. As discussed in the meeting to make the battery electrode, the functionalized porous silicon membrane will be prepared by Manipal University Jaipur. The ferrate nanoparticle will be prepared by SRM University and Flinders University. The characterization of studying the energy storage capacity will be carried out at Flinders University. In addition to this the Manipal University will synthesis the metal nanoparticles, titania and porous titania nanostructures. The porous silicon membrane along with metal nano-crystal will be used to study the photo catalysis process to generate hydrocarbon. The

photocatalysis study of prepared system will be carried out at Adelaide University Adelaide. The surface characterization will be carried out at Flinders University.

Proposed research work on Bi-functional Photocatalyst

Currently Flinders University is preparing Au cluster and understanding the interaction of this cluster with Titania nanoparticles. University of Adelaide is trying to find a best possible hetrostructure, Au cluster/Titania nanoparticles for production of hydrocarbon using CO_2 and H_2O. As a support of this hetrostructure glass is being used. SRM University will synthesis the Pt/Ru based clusters, Titania nanoparticles and the hetrostructure. University of Adelaide will do the study of heterogeneous catalytic reactions and Flinders University will study the surface property and stability. Manipal University Jaipur will make porous silicon membrane for the support and also it can be used for host surface of the metal cluster. The SRM University and University of Adelaide will jointly study the metal cluster, interaction energy and catalytic reaction mechanism using density functional theory and post-DFT.



Flowchart demonstrates the work plan during next six month, under the collaborative research work. Here M_c and MO_n denoted the metal cluster and metal oxide nanostructures respectively.

Annexure IV

Facility visited at University of Adelaide

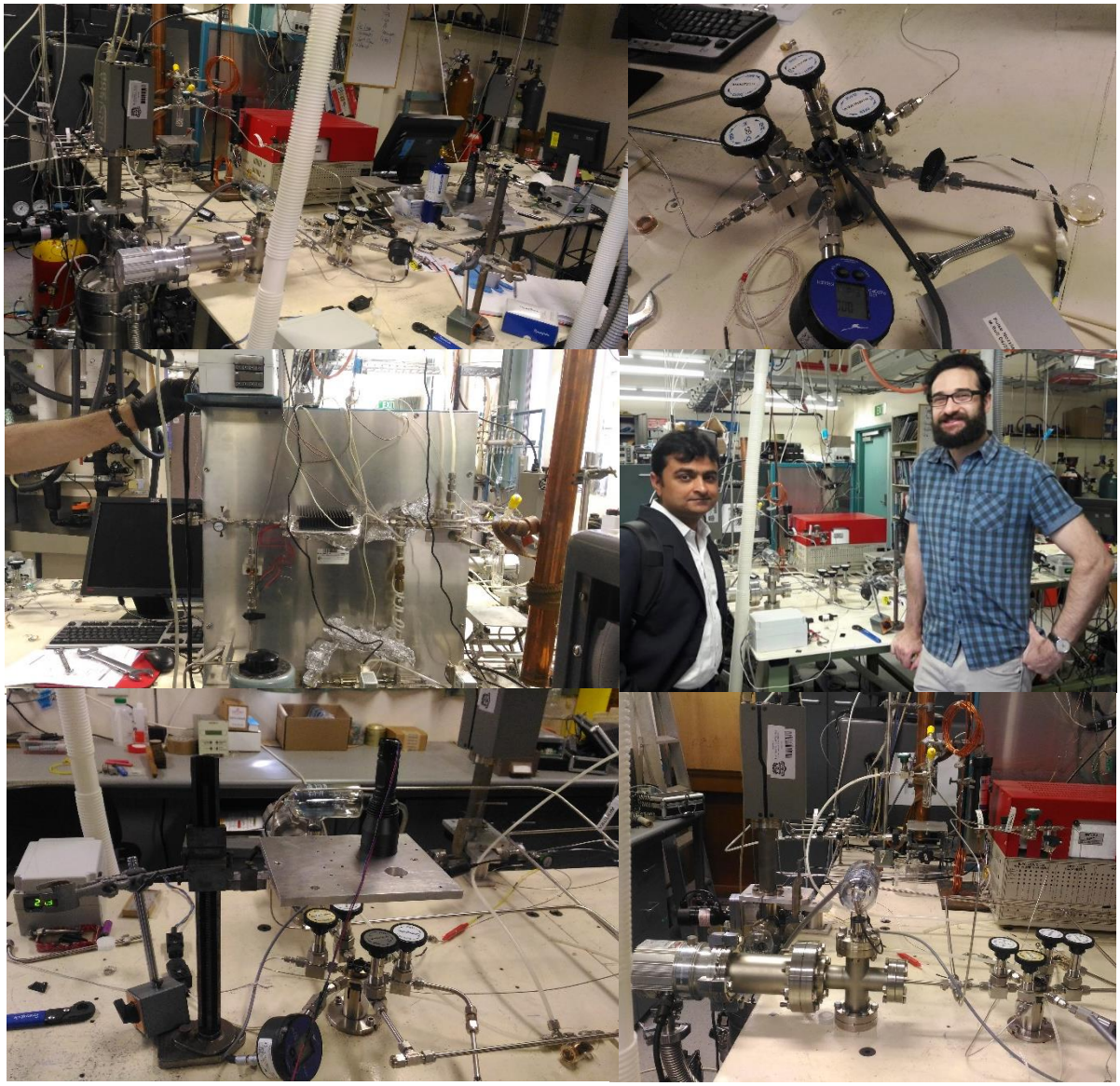


Photo 17. Lab based Setup for testing and analyzing various catalytic reactions using Hetrocatalyst. It is capable for CO oxidation, CO_2 hydrogenation, water gas shift reactions and other important reactions.

Prof. Greg is mainly interested in chemical and physical properties of nano and sub-nano metallic particles. Laser ablation techniques are used to generate metal cluster molecules in gas and solution phases. Various spectroscopic methods are elucidating their structures and properties, particularly chemical reactivity. They also apply quantum computational methods to calculate structures and properties of nano-scale

particles. His group is using density functional theory and density functional theory based tight binding approximation for estimating the properties of metal cluster.

The density functional based tight binding (DFTB) method is based on expansions of the Kohn-Sham total energy in density functional theory (DFT) with respect to charge density fluctuations. Furthermore, by self-consistent redistribution of charges (SCC), DFTB can be successfully applied to problems, where deficiencies within standard tight binding approach become obvious. As a result, fairly accurate simulations of large systems and longtime scales can be achieved with DFTB.

The main discussion with Prof. Greg and his group members is on synthesis of metal nanoparticles on TiO_2 nanostructures and using this hetrostructure as bi-functional catalyst. Also the theoretical verification using density functional theory was main topic of discussion.

He is also interested on the development of silicon pores membranes as support of the bi-functional catalyst. This can help the easy flow of reactant and product (in the form of gas) during catalytic measurements.