IITB-Monash Research Academy

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Project Title:	Development of high performance Li-S cell via designing/engineering of cathode and membrane with the use of new and improved nanomaterials	
Project Number	**IMURA0793**	
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Research Clusters: / Research Themes:

Highlight which of the Academy's CLUSTERS this project will address? *(Please nominate JUST **one.** For more information, see www.iitbmonash.org)*		**Highlight which of the Academy's Theme(s) this project will address?** *(Feel free to nominate more than one. For more information, see www.iitbmonash.org)*	
1	*Material Science/Engineering (including Nano, Metallurgy)*	3	*Clean Energy*
2	*Energy, Green Chem, Chemistry, Catalysis, Reaction Eng*	5	*Nanotechnology*
3	*Math, CFD, Modelling, Manufacturing*		

The research problem

Advanced and sustained electrochemical energy storage (EES) technology is deemed as one of the most promising avenues to address the ever increasing concerns associated with depletion of fossil fuel and rising levels of environmental pollution. Among the advanced EES, Li-ion battery system has been the most sought after technology. In the context of further enhancing the energy density of EES technology, Li-S battery is emerging as the most promising alternative [1]. The energy density of the Li-S system, having Li metal as anode and S as cathode, is expected to be greater than that of the more conventional Li-ion battery system (having graphitic carbon anode and transition metal oxide cathode) by factor of ~6 primarily due to the significantly higher Li-storage capacities of the electrode materials on both the sides. However, the extremely poor cyclic stability of the present generation Li-S cells, in addition to the considerably lower energy and power densities (as compared to those expected theoretically), has hindered the progress of Li-S system beyond the laboratory scale research and development [1,2].

The above drawbacks are primarily associated with the insulating nature of S, thus rendering the S utilization and kinetics of the electrochemical reaction dependent considerably on the nature/properties of the conducting backbone hosting the S. This also leads to the necessity of having inactive or 'dead' weight on the cathode side. More importantly, the polysulphides that form upon lithiation of S are soluble in the liquid organic electrolytes used and hence shuttle towards the Li anode; thus passivating/poisoning the same and also reducing the amount of active S available in the cathode with time. While the former negatively affects the energy and power densities, the later leads to the extremely poor cyclic stability (*viz.*, capacity retention over multiple discharge/charge cycles). To address the above issues, many electronically conducting materials, that possess high specific surface area (for forming multiple interfaces with S), have a considerable volume of nanosized porosities (*viz.*, meso/micro-porous materials) and also preferably possess the ability to 'bind' the polysulphides (*viz.*, having negative binding energies for S and Li) that form during lithiation, are used as S 'hosts'/'traps' at the cathode side [1]. In the last few years considerable attention has been devoted towards identifying and developing the best possible polysulphide 'trapping' materials on the basis of their electronic conductivities, binding abilities and optimized combinations of pore sizes/volumes; however, with limited long term success [1]. Some of the materials that have been at the forefront as the S 'hosts'-cum-'traps' include activated carbons and reduced graphene oxides (rGOs) [1,2]; with 2D materials like graphene, phosphorene, silicene, etc. also being investigated more recently due to their ability to bind with the polysulphides [3,4].

In addition to the conducting 'hosts'/'traps' as part of the cathode structure, a new concept has been proposed by Shaibbani et al. [5] (from Monash University, Australia), which uses an additional membrane made of graphene oxide and suitably 'placed' on 'top' of the S-containing cathode to further immobilize the polysulphides against getting lost from the cathode and depositing on the Li anode. Such innovative design and careful selection/optimization/engineering of the concerned materials led to considerable improvements in the cyclic stability of the as-developed Li-S cells. It is to be noted that the membrane design has to be such that it provides least possible hindrance towards the ionic transport through the electrolyte. Even though this was also taken care of via careful engineering, there is scope for still improving this aspect via further optimizations and engineering, along with improving the conductivity aspect of the aforementioned membrane. Overall, further improvements in the power density and also cyclic stability of the Li-S system, in light of the otherwise promising design as proposed by Shaibbani et al. [5], is envisaged by the usage of nanomaterials that can bestow improved electronic conductivity of such membrane (as also of the 'actual' S-containing cathode) and further improved capability of binding with the polysulphides. Identifying such materials, tuning them further in the context of the concerned usage and applying them in a carefully engineered manner to lead to the best possible improvement in the performances form the core of the proposed research.

References

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3. F. Li, J. Zhao, *ACS Appl. Mater. Interfaces* 2017, **9**, 42836.

4. J. Sun, H. -W. Lee, M. Pasta, H. Yuan, G. Zheng, Y. Sun, Y. Li, Y. Cui, *Nature Nanotech.*, 2015, **10**, 980.
5. M. Shaibani, A. Akbari, P. Sheath, C. D. Easton, P. C. Banerjee, K. Konstas, A. Fakhfouri, M. Barghamadi, M. M. Musameh, A. S. Best, T. Rüther, P. J. Mahon, M. R. Hill, A. F. Hollenkamp, M. Majumder, *ACS Nano* 2016, **10**, 7768.

Project aims

Against the above backdrops, the proposed research aims at identifying materials (and combinations) that would possess improved potential towards absorbing the Li-polysulphides (as formed upon lithiation with S cathode), as well as superior electronic conductivities. Such materials/combinations will be further tuned/optimized in the context of usage as part of the hosts or 'traps' for the S and Li-polysulphides in the cathode and/or in the membrane placed adjacent to the cathode. This will be followed by developing the S containing cathode and the membrane in a carefully engineered manner to allow the best possible utilization of such materials; eventually leading to the development of Li-S cells with the issues pertaining to the continuous loss of S (active material) from the cathode with discharge/charge cycles, passivation/poisoning of the Li anode and the rate capability of such electrodes addressed to the best possible extent.

Expected outcomes

Addressing of the aforementioned issues associated with the otherwise promising Li-S system via innovative and careful materials selection-cum-design is expected to allow the development of Li-S cells possessing power densities and cyclic stabilities that are superior with respect to the state of the art; thus contributing significantly towards the goal of significantly enhancing the energy density of the electrochemical energy storage technology, but without sacrificing on the cycle life and power density.

From a more scientific/learning perspective, the proposed research will lead to the understanding of various aspects related to physics and chemistry of nanomaterials, engineering of such nanomaterials to suit the desired application, the detailed electrochemical phenomena/approach involved and functioning/development of electrochemical energy storage system (which is among the major scientific-cum-societal necessities of the present day world).

How will the project address the Goals of the above Themes?

In a broader perspective, the presently proposed project is based on application of **nanomaterials** (such as layered 2D materials like graphene, possibly also phosphorene or silicene) and **nanotechnology** (such as development of multi-layered films, membranes of nanosized scales, engineering at the 'nano-level', electrochemical-mechanical *in-situ* studies with nanostructured materials and interfaces etc.) towards improvements in the electrochemical **energy storage** technology. In other words, contributing significantly towards the developments of **sustainable** energy storage technology. Such concerned improvements (based on the overall objective of the project) are essential for rendering the energy storage technologies suitable for applications related to development of *electric vehicles*, storing of energy 'harvested' from renewable sources like *solar energy* (which are needed for *controlling environmental pollution* and also in light of the *depletion of fossil fuels*) and *grid energy storage* (which is needed for allowing the large scale usage of the *cleaner*, but intermittent, *renewable sources of energy* like solar and wind) in a relatively economical-cum-sustainable manner. Finally, a key aspect of this project is to work along the lines of correlations between the physics/chemistry of nanomaterials, engineering of nanomaterials, electrochemical materials science and device fabrication; leading to the desired goal of significantly contributing towards the electrochemical energy storage technology.

Capabilities and Degrees Required

The student should ideally have a basic degree in areas related to Materials Science (including chemistry or physics) and/or Materials/Metallurgical Engineering (including Ceramic/Polymer Engineering). Candidates possessing good experimental skills and analytical, as well as thinking, ability will be preferred. Candidates having a CPI of > 7.5/10 (or overall % of 75%) in the qualifying examination/degree are likely to get preference. On a similar note, candidates having some previous research experience during Master's program or as research/project associate might get preference.

Potential Collaborators

Prof. Rajiv Dusane (Metallurgical Engineering and Materials Science, IIT Bombay), Prof. Sagar Mitra (Energy Science and Engineering, IIT Bombay), Prof. M. Aslam (Physics, IIT Bombay) and Prof Douglas R. MacFarlane (School of Chemistry, Monash)

Select up to **(4)** keywords from the Academy's approved keyword list **(available at http://www.iitbmonash.org/becoming-a-research-supervisor/)** relating to this project to make it easier for the students to apply.

Energy, Energy Storage, Energy Materials ;
Nanotechnology, nanoscience ;
Novel Batteries and Fuel Cells;
Modelling and Simulation