Project Title: Graphene exfoliation and nanohybrid formation for advanced Li-battery Cathode Material development

Project Number: IMURA608

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Research Academy Themes:
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. Advanced computational engineering, simulation and manufacture
2. Infrastructure Engineering
3. Clean Energy
4. Water
5. Nanotechnology
6. Biotechnology and Stem Cell Research

The research problem:
Currently, the specific capacity of commercialised lithium ion battery (LIB) is limited by its current cathode material, LiFePO₄, in which its theoretical capacity limit of 170 mAh/g has already been reached. In order to circumvent this limitation, there is a constant search for the next generation cathode materials that can deliver the coveted high energy densities. Amongst them, lithium metal silicates (Li₂MSiO₄) are very promising due to the elemental abundance of silica, low cost and high theoretical specific capacity of 330.
mAh/g. However, the highest reported capacity based on mixed metal silicates (Li\textsubscript{2}Mn\textsubscript{x}Fe\textsubscript{1-x}SiO\textsubscript{4}) was only 250 mAh/g due to difficulties in the complete extraction of the two Li ions. Furthermore, the quality of the energy obtained was poor as the voltage profiles were steeply sloping over a wide range (4.5–1.0 V versus Li/Li\textsuperscript{+}) which may be partly due to the severe kinetic and electronic limitations of the materials. There have been attempts with nanostructuring strategies and applying conductive carbon coatings but the full potentials of these next generation materials have yet to be realised.

**Project aims**

*The aim of this work is to produce the graphene-Li\textsubscript{2}MSiO\textsubscript{4} nanohybrids electrochemically (as opposed to the more established wet chemical synthesis), so as to integrate and streamline the electrochemical production process from graphite exfoliation to the formation of highly value-added nanohybrids, all in one step. The electrochemical synthesis process is expected to be cost-effective and highly beneficial to the selective growth of crystal phase which will facilitate the electrochemical intercalation and extraction of lithium ions. Ultimately, tuning of the electronic structure of the graphene scaffold can be achieved by functionalisation or doping to influence the electrochemical activity of the cathode materials.*

**Expected outcomes**

*The key relies on the electrochemistry to form the right graphene-based nanohybrids and the success of this project will be realised by a number of key innovations:*

1. *The cost-effective electrochemical exfoliation of raw graphite flakes and tailoring of specific functional graphene functional groups through electrochemical functionalization can directly make new applications of graphene in the areas of electrochemistry possible. It is a platform technology that can produce a huge variety of functional materials.*

2. *The central theme focuses on devising a direct electrochemical synthesis of graphene-based nanohybrids to directly transform graphite into functional graphene-based materials (beyond the production of functionalised graphene), hence bypassing many synthetic steps involved in current graphene-based multicomponent nanohybrid technology. Not only can it provide a straightforward and cost-effective solution, it can also deliver a synergistic effect due to the unique chemical bonding between target of interest and graphene, which might otherwise be difficult to achieve with traditional chemical reactions.*

3. *Due to the nature of electrochemical synthesis, good electrical connectivity between the nanohybrids, themselves and the current collector during the electrochemical-directed growth is realised. Furthermore, the porosity of the graphene-based nanohybrids can also be tuned via the electrochemical parameters or electrolyte additives, and that will greatly influence the lithium ion transport in the cathode material.*

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

*NanoTechnology – The project will deliver the superior LiBs with graphene-based nanohybrids.*
Capabilities and Degrees Required

- Chemistry as major with sound knowledge in inorganic material synthesis, electrochemistry and solid-state chemistry
- Chemical Engineering with relevant experience in materials synthesis and characterization are must
- Materials Science with relevant experience in materials synthesis and characterization are must

Potential Collaborators

Please visit the IITB website www.iitb.ac.in OR Monash Website www.monash.edu to highlight some potential collaborators that would be best suited for the area of research you are intending to float.

Please provide a few key words relating to this project to make it easier for the students to apply.

Graphene, Nanotechnology, Energy Storage