IITB-Monash Research Academy

Indian Institute of Technology Bombay | MONASH University

An Indian-Australian research partnership

Project Title:	'Layered' transition metal oxide cathode material for Na-ion batteries: from fundamentals to prototype development	
Project Number	**IMURA1064**	
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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)*** √	***1***	*Artificial Intelligence and Advanced Computational Modelling*
2	*Energy, Green Chem, Chemistry, Catalysis, Reaction Eng*	2	*Circular Economy*
3	*Math, CFD, Modelling, Manufacturing*	3	***Clean Energy*** √
4	*CSE, IT, Optimisation, Data, Sensors, Systems, Signal Processing, Control*	4	*Health Sciences*
5	*Earth Sciences and Civil Engineering (Geo, Water, Climate)*	5	*Smart Materials*
6	*Bio, Stem Cells, Bio Chem, Pharma, Food*	6	*Sustainable Societies*
7	*Semi-Conductors, Optics, Photonics, Networks, Telecomm, Power Eng*	7	*Infrastructure*
8	*HSS, Design, Management*		

The research problem

Scarcity of Li- and Co-resources, both of which have global supply chain issue, along with the ever-increasing demand for sustainable and cost-effective energy storage system, mandates the development of battery systems which can harness abundant minerals and resources. Na-ion battery system which in addition to the above benefits can eventually match the performance of the Li-ion battery system, benefitting from significant research developments. In fact, Na-ion battery system is a fast-growing market with a current market share of more than 40%, as the ubiquitous abundance of Na-resources makes it a lone choice for commercial penetrance.

Cathode materials dictate the performance of alkali metal-ion cells (such as Na-ion cells) to a significant extent and are the alkali metal ion reservoirs in such cells (*viz.*, Na-reservoir in Na-ion cell). Even though 'layered' Na- transition metal (T_M) oxides are deemed to be the most suitable class of material for usage as cathode materials in the upcoming Na-ion battery system, they suffer from loss in structural integrity upon electrochemical Na-extraction/insertion (*i.e.*, charge/discharge of cell) and instability upon being exposed to air/moisture [*J. Mater. Chem. A* **8** (2020) 18064-18078]. While the former leads to drastic fade in Na-storage capacity upon being used for charge/discharge cycles, the latter renders handling/storage challenging and also make it rather mandatory to use hazardous/expensive chemicals like N-methyl pyrrolidone (NMP) (instead of water) for electrode processing. Furthermore, despite being the Na-reservoir of the cell, the 'layered' Na-T_M-oxides are often Na-deficit in the as-synthesized conditions [*Chem. Mater.* **34**[23] (2022) 10470–10483].

Against these backdrops, the proposed research first aims at addressing the above problems by designing a suitable composition for the 'layered' Na-T_M-oxides so that they possess the desired structural features and, thus, exhibit vastly improved air/water-stability and electrochemical stability, along with high Na-storage capacity. This will be primarily aided by suitably tuning the overall covalency of the T_M-anion bond by careful selection of the cations in the T_M-layer and possible partial substitution of O-ion with other anions (to be done primarily at IIT Bombay). Once the above material-related aspects are addressed and good performances achieved at Na 'half' cell level by also addressing possible issues at electrode/electrolyte interface (at IIT Bombay), the as-designed high-performing cathode material will be taken forward towards development of Na-ion 'full' cells, first in coin cell format, followed by larger capacity pouch cell format, as a laboratory-scale prototype (to be done primarily at Monash University).

Project aims

The proposed research aims at developing high-performance and novel 'layered' Na-T_M-oxide based cathode materials for Na-ion batteries, possessing the desired composition and structural features that will help address the major problems related to instabilities upon exposure to air/water and electrochemical cycling (to be done primarily at IIT Bombay).

The development of the novel cathode material will be followed by optimizing the cathode/electrolyte interface, primarily by way of suitably tuning the electrolyte formulation, leading to excellent cyclic stability in coin cell format (to be done primarily at IIT Bombay).

Following this, the research will result in the development of Na-ion 'full' cells based on the as-developed cathode, first in coin cell format (at IIT Bombay and Monash University) and then in larger capacity pouch cell format, as a laboratory-scale prototype (to be done primarily at Monash University).

What is expected of the student when at IITB and when at Monash?

At IIT Bombay, the student will be working on the materials and electrochemical aspects (*viz.*, primarily the associated science) of ‘layered’ Na- transition metal oxides to lead to the development of a high-performance cathode material for the upcoming Na-ion battery system. Following this, at Monash University, the student will be involved with the fabrication of Na-ion ‘full’ cell at a larger format and addressing of the engineering issues that come in the way towards achieving the desired performance metrics.

Expected outcomes

From the deliverable perspective, the proposed project will lead to the development air/water-stable and electrochemically stable high-voltage, high-capacity Co-free ‘layered’ Na-T_M-oxides as cathode materials for Na-ion battery system. The targets will include Na-storage capacity of > ~150 mAh/g, along with minimal impedance and excellent long-term cyclic stability (~80% capacity retention up to ~500 cycles). Eventually, the best performing cathode will be used for the fabrication of high-voltage/capacity and electrochemically stable Na-ion ‘full’ cells in the pouch cell format.

From the fundamental perspective, the proposed research will lead to new understandings on the effects of electronic configuration of T_M-ions and non-T_M-ion dopants towards crystallographic site occupancy, T_M-O bond covalency, differential dilation/shrinkage of T_M-‘slab’/Na-‘inter-slab’ spacings in lattice; and influences of the above towards water-stability and structural/phase transformations during Na-removal/insertion. On a broader perspective, this will throw new insights into the above aspects of Na-T_M-oxides as a class of material; which may be useful even beyond electrochemical energy storage.

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

The project will contribute to the development of cost-effective, sustainable and high-performance electrochemical energy storage system in the form of Na-ion batteries, which is likely to eventually match the performance of (and possibly outperform, as well) the relatively less sustainable and more expensive Li-ion battery system in a variety of applications, including storage of energy harvested from the clean/renewable sources and grid energy storage. With further research, as proposed here, Na-ion battery systems may find applications even in electric vehicles and, thus, provide further impetus towards the development-cum-commercialization of the same. It may be recalled here that the scarcity of Li- and Co-resources, both of which are unavailable in India, along with the ever-increasing demand for sustainable and cost-effective energy storage system, mandates the development of Na-ion battery system (*viz.*, in the context of societal need). Hence, the proposed research is likely to contribute, in significant terms, towards the ‘Clean Energy’ theme of the Academy. In the past few years India has seen significant investment into battery manufacturing, but it is also clear that the infrastructure including man-power, know-how and intellectual capital required to sustain this growing industry requires major investment and attention. The project, while being, small and focussed attempts to address this new surge of man-power requirement.

Potential RPCs from IITB and Monash

Faculty members having expertise in battery materials/interfaces, such as Prof. Srinivasan Ramakrishnan, from Chemistry Department, IIT Bombay; and Prof. Douglas McFarlane from Monash University, may be considered as potential RPC members.

Capabilities and Degrees Required

The candidate is required to have at least one of the following academic backgrounds, as part of the Bachelors or Masters' program undertaken; *viz.*, Materials Science/Engineering or related, Ceramic Engineering, Chemistry and Physics.

Any prior experience with battery related work may be an added advantage, but not at all mandatory.

Necessary Courses

The student may be advised to do courses related to Structure of Materials, Materials-Electrochemical Perspectives in Energy Storage, Electrochemical Reaction Engineering, Materials Thermodynamics etc.

Potential Collaborators

Collaborators who might be able to help with atomic resolution HAADF-STEM imaging (in TEM), Synchrotron based characterizations and solid-state NMR based characterizations may help further.

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 materials, energy storage, green chemistry and renewable energy, electrochemistry, transition metal oxides