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| **Topic:** | **Computational Materials Design for Next Generation Rechargeable Batteries** |
| **Speaker:** | **Dr. Nikhil V. Medhekar**<br>Department of Materials Engineering, Monash University, Australia |
| **Date:** | **2 October 2014, Thursday** |
| **Time:** | **2.00pm to 3.00pm** |
| **Venue:** | **EA-02-11** *(map of NUS can be found at http://map.nus.edu.sg/)* |
| **Host:** | **Dr. Sergei Manzhos** |

## Abstract

Lithium ion batteries are today's state-of-the-art energy storage technologies. Due to high volumetric and energy densities, they have become the industry standard for portable applications such as consumer electronics and hybrid vehicles. However, lithium ion batteries also have large capital costs, which make them prohibitively expensive for grid-based energy storage. Therefore, there is a clear need for new innovative energy storage systems which are able to meet the required performance standards as well as the necessary economic benchmarks that make them commercially viable. Compared to lithium ion batteries, sodium ion batteries provide a very attractive low cost alternative for stationary energy storage systems where battery size and weight are not the most crucial design constraints. However, establishing suitable electrode chemistries for Sodium ion batteries remains a crucial challenge. In this talk, I will highlight our group's recent work on identifying suitable electrode materials for sodium ion batteries using advanced computational techniques. We considered two classes of materials, namely sodium-metal alloys and transition metal dichalcogenides and oxides, as representative materials for anode and cathodes in sodium ion batteries. We characterised fundamental electrochemical characteristics of these materials for Sodium intercalation as well as their intercalation-induced mechanical behaviour. Our analysis essentially establishes the electrochemical performance of these materials as well as their viability as electrodes in sodium ion batteries.

**References:**

M. Motazavi, J Deng, V. B. Shenoy and N. V. Medhekar, "Elastic softening of alloy negative electrodes for Na-ion batteries", J. Power Sources 225, 207 (2013).

M. Mortazavi, C. Wang, J. Deng, V. B. Shenoy and N V. Medhekar, "Ab initio characterization of sodium intercalation in layered transition metal dichlcogenides", J. Power Sources 268, 279 (2014).

M. Mortazavi, N. Birbilis and N. V. Medhekar, "High capacity group 15 alloy negative electrodes for Na-ion batteries: electrochemical and mechanical insights", in review (2014).

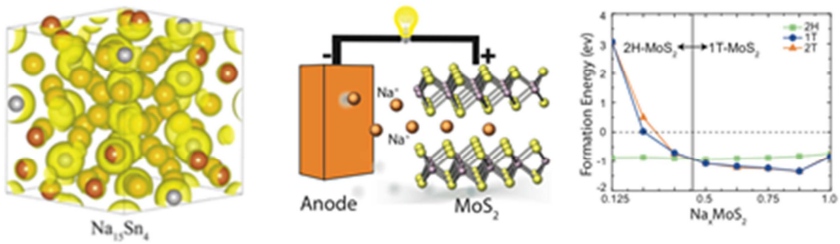


**Figure:** (a) Electronic structure of Sodium intercalated crystalline tin [1], (b) Thermodynamics of sodium intercalation in layered transition metal dichlcogenides [2].

## About the Speaker

Dr Nikhil Medhekar is a senior lecturer at the Department of Materials Engineering at Monash University. He received his PhD degree at the Division of Engineering at Brown University, USA, in 2009, specializing in Mechanics of Solids and Structures. Prior to joining the graduate studies at Brown University, he earned his Masters of Technology in Mechanical Engineering at the Indian Institute of Technology, Bombay; and worked as a Mechanical Engineer at the General Electric Corporate Research Center. Dr Medhekar is a recipient of the Materials Research Society's Graduate Student Award for the year 2008. In 2010, he moved to Monash University, where he leads the Computational Materials Laboratory.

**Admission is free. All are welcome to attend.**