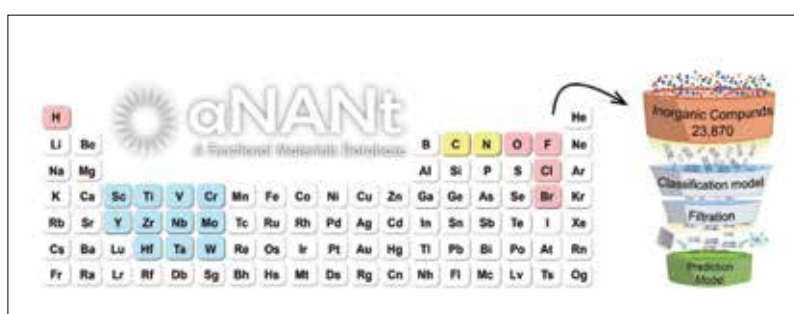# DIVISION OF
Chemical Sciences
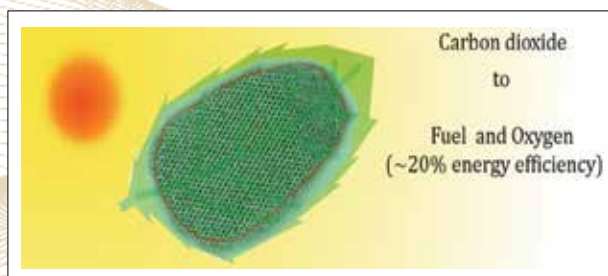
RESEARCH SNAPSHOTS 2018

ABHISHEK SINGH (MRC)

The application of machine learning (ML) to develop structural and functional materials is relatively new, however, has great potential to accelerate the discovery of materials for a desired application. A foremost requirement in designing predictive models is the availability of high quality scientific data in the form of shared materials databases. Continuous update and establishment of new databases are crucial for targeted applications. In this regard, Materials Theory and Simulations Group at Materials Research Centre has developed an open-access online repository of functional materials. The database is called aNANt and hosts the structures and electronic properties of more than 10000 functionalized MXene. It is expected to grow to host 25000 functionalized MXene within few months. Using information from this database, we have recently developed a ML model to predict the accurate band gap of functionalized MXene.

Reference: Rajan, A. C.; Mishra, A.; Satsangi, S.; Vaish, R.; Mizuseki, H.; Lee, K. R.; Singh, A. K. Chem. Mater.2018 In press.
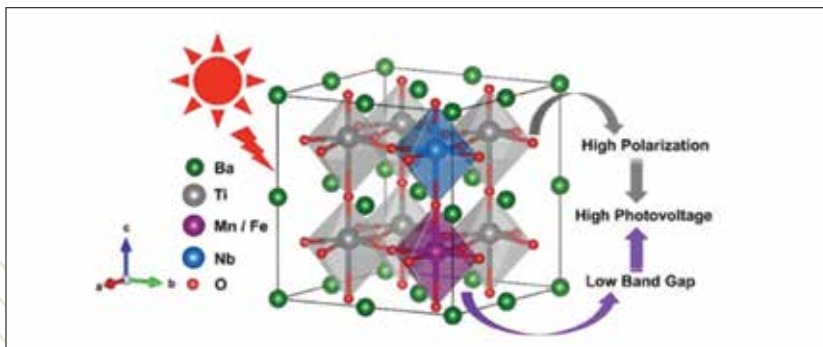

ANSHU PANDEY (SSCU)

Artificial photosynthesis is a very promising idea, since it can directly help capture atmospheric carbon dioxide and convert to a fuel or an industrial feedstock. While extensive efforts have been made towards electrically assisted CO_2 reduction, exclusively photocatalytic reduction remains in a relatively nascent state. In this work we have designed and prepared $CuAIS_2/ZnS$ quantum dots that can reduce aqueous bicarbonate ions to formate under visible light. We are able to get high turnover numbers (>7÷Đ10Đ^4 molecules of sodium formate produced per quantum dot) and also solar to chemical energy conversion efficiencies as high as 20%. This efficiency is roughly 100 times greater than what is typically achieved in natural photosynthesis.

Reference: Bhattacharyya, B.; Simlandy, A. K.; Chakraborty, A.; Rajasekar, G. P.; Aetukuri, N. B.; Mukherjee, S.; Pandey, A. Efficient Photosynthesis of Organics from Aqueous Bicarbonate Ions by Quantum Dots Using Visible Light. ACS Energy Lett. 2018, 3, 1508-1514
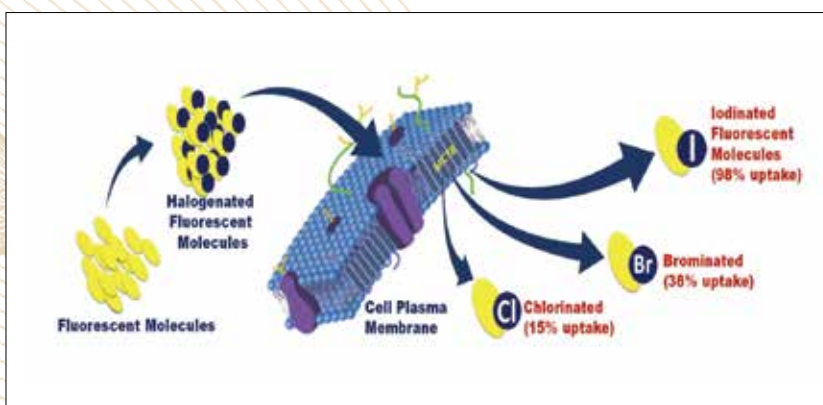
D D SARMA (SSCU)

Any ferroelectric material is potentially an efficient solar energy converter. Unfortunately, all known ferroelectric materials have large band gaps with little overlap with the solar spectrum and therefore, poor ability to absorb and convert sunlight to electricity. We recently discovered an efficient way to reduce the band gap of a classical ferroelectric material, $BaTiO_3$, without compromising its ferroelectric polarization significantly with the help of a charge-neutral dipole doping of Mn^{3+}-Nb^{5+} pair replacing two Ti^{4+} ions.

Reference: Shyamashis Das, Somnath Ghara, Priya Mahadevan, A. Sundaresan, J. Gopalakrishnan, and D. D. Sarma; Designing a Lower Band Gap Bulk Ferroelectric Material with a Sizable Polarization at Room Temperature ACS Energy Lett. 2018, 3, pp 1176–1182; (DOI: 10.1021/acsenergylett.8b00492)
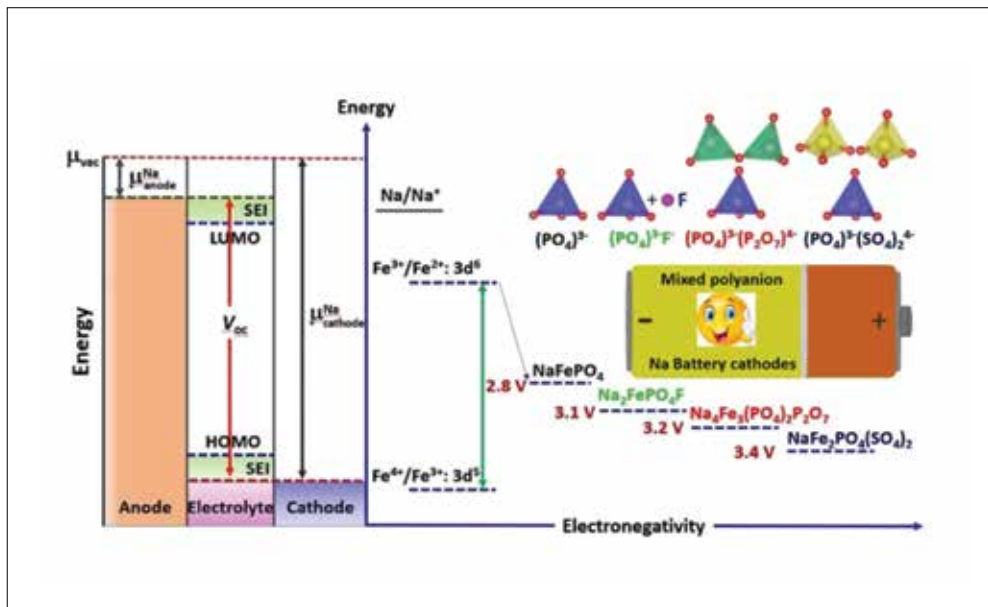

G. MUGESH (IPC)

For decades, scientists have used fluorescent probes to detect molecules, monitor cellular activity and deliver drugs inside cells. Probes based on a compound called naphthalimide are especially popular because they can easily be made in large quantities and their fluorescence can be tweaked by changing their constituent atoms. But they are usually absorbed by cells only in small quantities, which hampers their effectiveness. In addition, little is known about how they cross the cell membrane to reach inside.

In a new study, researchers from the Indian Institute of Science (IISc) have figured out a way to boost the cellular uptake of such fluorescent probes. They found that simply replacing two hydrogen atoms with iodine in their structure dramatically increases the amount transported into mammalian cells – up to 98%.

Reference: The Remarkable Effect of Halogen Substitution on the Membrane Transport of Fluorescent Molecules in Living Cells, published in AngewandteChemie International Edition, May 2018.https://onlinelibrary.wiley.com/doi/abs/10.1002/anie.201804128
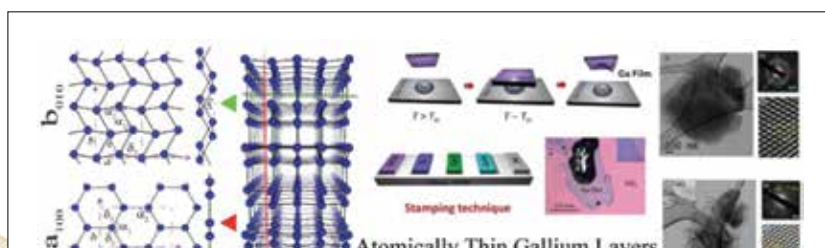
PRABEER BARPANDA (MRC)

'Building better batteries' remains an ongoing process to cater diverse energy demands starting from small-scale consumer electronics to large-scale automobiles and grid-storage. While Li-ion batteries have carried this burden over the last three decades, the ever-growing and highly diverse applications (based on size, energy-density and stationary vs. mobile usages) have led to an era of 'beyond lithium-ion batteries'. In this post-lithium-battery genre, sodium-ion batteries (NIBs) have emerged as a pragmatic option particularly for large-scale applications. Our current work focuses on the world of mixed polyanionic cathode materials to realize the next generation sodium-ion batteries with high energy density.

Reference:: P. Barpanda et al, Adv. Energy Mater, 8(27), 1703055, 2018.

ABHISHEK SINGH (MRC)

Gallium, with its rich low-temperature phase diagram, is a liquid metal at room temperature and displays impressive potential for use as a 2D material. Theoretical and experimental investigation by groups of A. K. Singh at IISc and P. M. Ajayan at Rice University, USA introduce a new approach for realization of thin 2D sheets of gallium, called as "gallenene".

Reference: Kochat*, A. Samanta*, Y. Zhang, S. Bhowmick, P. Manimunda, S. A. S. Asif, A. Stender, R. Vajtai, A. K. Singh, C. S. Tiwary, P. M. Ajayan, Atomically thin gallium layers from solid-melt exfoliation Science Advances , 4, e1701373 (2018).