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Pseudo-2D to Real-Two Dimensional Nanostructures: Their Use in High Performing Energy Storage Devices

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Abstract

Metal oxides, with various particle morphologies, are widely used in batteries and supercapacitors. Mostly, solid particles of metal oxides having different compositions, crystal structure, porosity, surface area and thermal stability were investigated. The discovery of graphene changed the scenario. There has been an avalanche of papers, where 2D materials are being reported for high performing energy storage. Additionally, over the last few years, a lot of interest has been generated by particles with hollow morphologies. These are particles of various shapes and sizes but with one common feature i.e. a cavity in the middle. These particles have routinely shown that, owing to their enhanced specific surface area, they have much higher electrochemical behaviour. It will be shown that this is an oversimplified explanation. If only the surface area was driving the enhancement then other solid morphologies, with higher specific surface area, should have shown better performance. Careful modelling and simulation studies by LAMMPS software shows that hollow structures actually simulate properties of 2-dimensional (2-D) like materials. This leads to performance similar to that reported in real 2-dimensional materials ranging from metal oxides to MXenes.

The second part of the talk will focus on sodium-ion batteries (NIBs) fabricated using real 2-D materials. Nitrogen doped carbon (NDC)_MoS₂ composite, as an anode material, is able to deliver excellent rate capability and long cycle life. It also delivers very high capacity of 1875 mAh g⁻¹ at 0.1 A g⁻¹. The full cell based on NDC_MoS₂ and sodium vanadium phosphate, as a cathode material, outperforms most reported studies. The battery delivers high specific capacity of 236 mAh g⁻¹ at 0.1 A g⁻¹ current density.

Finally, as move to technologies beyond lithium, I will give a brief overview on our recent work dealing with aluminium-ion batteries (AIBs).

Few select references:

Chandra et al.: *Nanoscale* 7, 19250 (2015); *Adv. Ener. Mater.* 8, 1800573 (2018), *CrystEngComm* 22, 1633 (2020), *ACS App. Ener. Mater.* 6, 753 (2023) and 5, 7735 (2022); *Mater. Adv.* 3, 5987 (2022); *J. Mat. Chem. A* 9, 6460 (2021)