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Electro-/Magneto-/Mechano-Active Smart Materials and Devices for Emerging Sensing and Storage in Railway Electrification Systems

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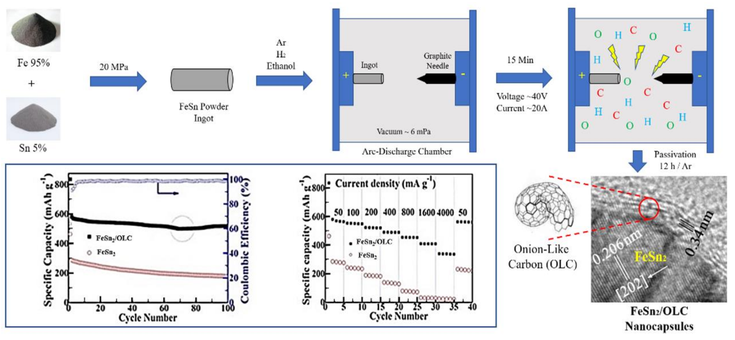
Project Summary

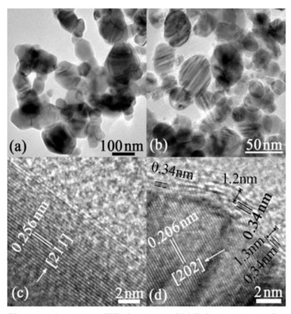
- The development of electro-/magneto-/mechano-active smart materials and devices technologies for emerging sensing and storage in railway electrification systems has been implemented in the present project to underpin the strategic development of both RGC–RIF (#R5020-18) and CNERC-Rail (#K-BBY1) projects.
- Four key and advanced types of smart materials, devices, and control techniques for sensing and storing of energies have been proposed and realized.
- These includes:
  1) An in-situ arc discharge-derived FeSn2/onion-like carbon nanocapsule as an improved stannide-based electrocatalytic anode for Li-ion batteries;
  2) A metal–organic framework-derived MnO/CoMn2O4@N–C nanorod with nanoparticle interstitial decoration in core@shell structure as a novel bifunctional electrocatalytic cathode for Li–O2 batteries;
  3) A self-assembled 3D macroscopic graphene/MXene-based hydrogel as an enhanced electrocatalytic electrode for supercapacitors; and
  4) A novel ensemble long short-term memory neural network model for improved remaining useful life prognosis of time-series sensor signals.
- Four good SCI journal papers have been published as the direct research output.
- The research results and the acquired knowhow will be applied to and further developed in the on-going RGC–RIF project and the coming CNERC-Rail project(s).

In-situ Arc Discharge-derived FeSn2/Onion-like Carbon Nanocapsules as Improved Stannide-based Electrocatalytic Anode for Lithium-ion Batteries

Published in Catalysts 9(11): 950, 2019

- Core/shell-structured $FeSn_2$/onion-like carbon ($FeSn_2$/OLC) nanocapsules are synthesized via an in-situ arc-discharge process to allow a facile one-pot procedure for forming a crystalline $FeSn_2$ stannide alloy nanoparticle core coated by a defective OLC thin shell, besides a confined crystal growth of the $FeSn_2$ nanoparticle cores in the sub-50 nm range.
- A formation mechanism is proposed to describe the confined crystal growth of the $FeSn_2$ nanoparticle cores and the formation of the $FeSn_2$/OLC core/shell structure.
- The nanocapsules are evaluated as an improved stannide-based electrocatalytic anode to extend the application scopes of Li-ion batteries (LIBs) to new energies and electric vehicles.
- The nanocapsule anode-based LIB cells exhibit enhanced electrochemical performance, including higher reversible capacity, better cyclability, and superior rate capability, in comparison with the $FeSn_2$ nanoparticle anode-based LIB cells counterpart.
- The observed electrochemical performance enhancement is ascribed to the synergetic effects of the enabling of a reversible lithiation process during the charge–discharge of the LIB cells by the $FeSn_2$ nanoparticle cores as well as the protection of the $FeSn_2$ nanoparticle cores from the volume change-induced pulverization and the solid electrolyte interphase-induced passivation by the OLC shells.



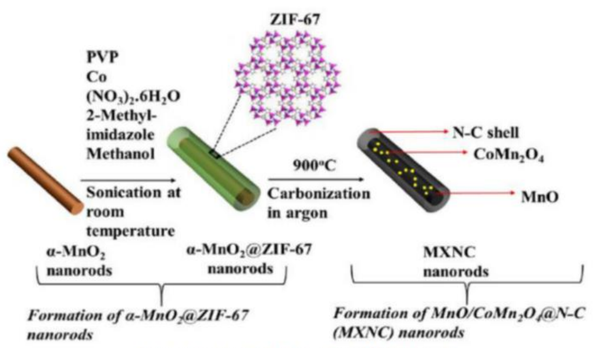


Transmission Electron Microscope (TEM) images of (a) $FeSn_2$ nanoparticles and (b) $FeSn_2$/OLC nanocapsules. HR-TEM images of (c) $FeSn_2$ nanoparticles and (d) $FeSn_2$/OLC nanocapsules.

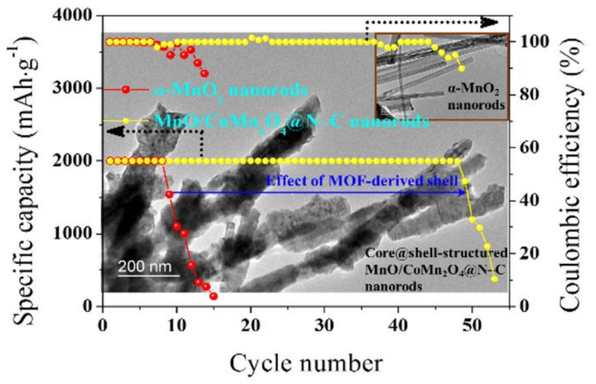
Metal–Organic Framework-derived MnO/CoMn2O4@N–C Nanorods with Nanoparticle Interstitial Decoration in Core@Shell Structure as Novel Bifunctional Electrocatalytic Cathode for Li–O2 Batteries

Published in Electrochimica Acta 338: 135809, 2020

- Core@shell-structured, hierarchically porous manganese oxide/cobalt manganite@nitrogen-doped carbon ($MnO/CoMn_2O_4$@N–C) nanorods with interstitially decorated $CoMn_2O_4$ nanoparticles are synthesized via one-step carbonization of metal–organic framework (MOF)-coated α-manganese oxide (α-MnO_2@ZIF-67) nanorods to exhibit a MnO nanorod core with $CoMn_2O_4$ nanoparticle interstitial decoration, both coated by an N–C conductive shell.
- The MnO core renders Mn active sites and O2 vacancies; the $CoMn_2O_4$ interstitial decoration gives additional Mn, Co active sites and enhances the bifunctional electrocatalytic ORR–OER; the N–C shell increases electronic conductivity, hierarchical porosity, specific surface area, and protects the core and interstitial decoration against lithium peroxide (Li_2O_2) passivation.
- The $MnO/CoMn_2O_4$@N–C nanorods are evaluated as a novel bifunctional electrocatalytic cathode for Li–O_2 batteries (LOBs) to improve the bifunctionality, specific discharge capacity, and cyclability of α-MnO_2 nanorod cathode-based LOBs.
- The improved structural features allow the $MnO/CoMn_2O_4$@N–C nanorod cathode-based LOB cells to exhibit superior full specific discharge capacity of 8,625 mAh·g^{-1} and cyclability of 48 discharge–charge cycles at 200 mA·g^{-1} specific current and 2,000 mAh.g^{-1} limited specific discharge capacity compared to their α-MnO_2 nanorod counterparts.
- Such MOF-derived, interstitial nanoparticle-decorated nanoarchitectures can lead to high-performance tunable bifunctional electrocatalysts and energy storages.



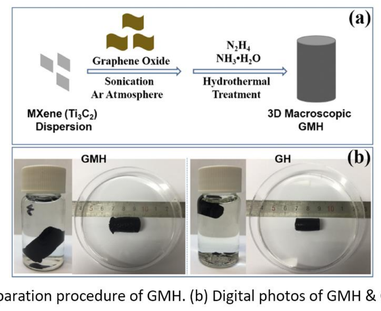
Schematic representation of the synthesis of MXNC nanorods.



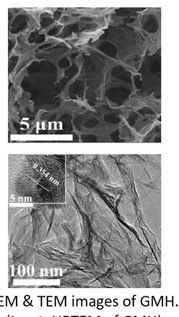
Self-assembled 3D Macroscopic Graphene/MXene-based Hydrogel as Enhanced Electrocatalytic Electrode for Supercapacitors

Published in APL Materials 8(9): 091101, 2020

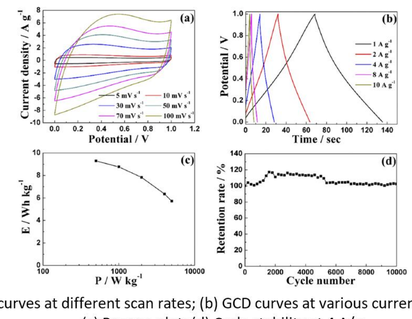
- A cylindrical-type 3D macroscopic graphene/MXene-based hydrogel (GMH) is prepared by self-assembling laminar-structured graphene oxide (GO) and MXene (Ti_3C_2) nanosheets via a facile one-step hydrothermal process.
- The GO is found to self-converge into a 3D macroscopic porous graphene framework during the hydrothermal process, while the Ti_3C_2 nanosheets are able to prevent the graphene nanosheets from self-restacking.
- The GMH shows a larger specific surface area of 161.1 m²/g and a higher pore volume of 0.5 cm³/g in comparison with the pure graphene hydrogel.
- A symmetric supercapacitor utilizing the GMH as electrodes exhibits high energy densities of 9.3 and 5.7 Wh/kg at different power densities of 500 and 5,000 W/kg, respectively, in addition to an outstanding long-term cycle stability with no loss in capacitance in excess of 10,000 continuous charge–discharge cycles.
- The proposed 3D macroscopic GMH is expected to realize promising high-performance hydrogel electrodes for new generation electrochemical energy storages.



(a) Preparation procedure of GMH. (b) Digital photos of GMH & GH.



SEM & TEM images of GMH. (Inset: HRTEM of GMH)

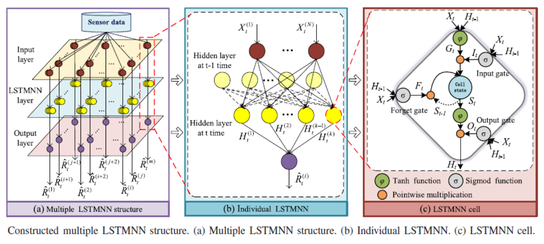


a) CV curves at different scan rates; (b) GCD curves at various current densities; (c) Ragone plot; (d) Cycle stability at 4 A/g.

Novel Ensemble Long Short-term Memory Neural Network Model for Improved Remaining Useful Life Prognosis of Time-series Sensor Signals

Published in IEEE Transactions on Instrumentation & Measurement 70: 3503912, 2021

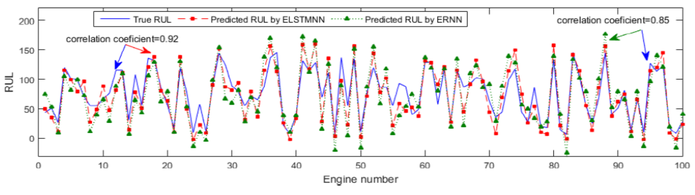
- A novel ensemble long short-term memory neural network (ELSTMNN) model is proposed for improving the remaining useful life (RUL) prognostic accuracy of time-series sensor signals as well as the adaptive and generalization abilities under different prognostic scenarios.
- The ELSTMNN contains a series of long short-term memory neural networks (LSTMNNs), each of which is trained on a unique set of historical data.
- A novel ensemble method is proposed using Bayesian inference algorithm to integrate multiple predictions of the LSTMNNs for the optimal RUL estimation.
- The effectiveness of the ELSTMNN-based RUL prognosis method is validated using two characteristically different turbofan engine data sets, and the experimental results show a competitive performance of the ELSTMNN in comparison with other prognostic methods.



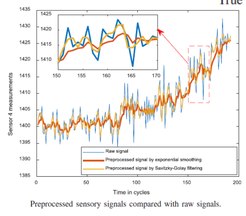
Constructed multiple LSTMNN structure. (a) Multiple LSTMNN structure. (b) Individual LSTMNN. (c) LSTMNN cell.

RUL Prediction Based on the ELSTMNN

Step 1:	Define a RUL prediction scenario and preprocess multi-sensor monitoring signals collected from multiple identical equipment after selecting appropriate sensor.
Step 2:	Use multiple LSTMNNs to learn fault evolution of different equipment in training dataset simultaneously.
Step 3:	An ensemble model is established based on the multiple evolved LSTMNNs integrated by BIA.
Step 4:	Evaluate the RUL prediction performance of ELSTMNN based on the test data.



True RUL versus predicted RUL for 100 engines in FD003.



Preprocessed sensory signals compared with raw signals.