Supporting Information

Hybrid Perovskite-like Iodobismuthates as Low-cost and Stable Anode Materials for Lithium-ion Battery Applications

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Experimental Section:

Synthesis of IMB, ADB and ATB powder.

For ATB and ADB, a 1:1 molar ratio of aminothiazolium iodide (or 2-amino-1, 3, 4-thiadiazolium for ADB) and bismuth iodide were dissolved separately in water (room temperature) and ethanol (60 ◦C) before mixing. The reaction was left for 3 hours before drying by a rotary evaporator. For IMB, a 3:2 ratio of imidazolium iodide and bismuth iodide was reacted with the same method above. The as-prepared powders were washed in diethyl ether followed by drying under vacuum.

Electrode fabrication:

Electrodes were fabricated by direct mixing of the active materials (Bi based materials), Super-P carbon and Polyvinylidene difluoride (PVDF) binder in a weight ratio of 7:2:1 in a minimum amount of N-methyl 2-pyrrolidine (NMP) solvent followed by coating the mixture onto a conducting Cu foil. It was then dried overnight in an oven at 80ºC. We note that Super P carbon does not contribute much to the capacity (~10-20 $mAhg^{-1}$) since the additive weight % is very low.

Coin cell fabrication:

2032 coin cells were fabricated using Li metal as one of the electrodes alongside celgard separators. Lithium hexafluorophosphate ($LiPF_6$) dissolved in 1:1 mixture of Ethylene Carbonate (EC) and Di-methyl Carbonate (DMC) with a 5% Fluoroethylene Carbonate (FEC) additive was used as the electrolyte. A total amount of 150 µl of electrolyte was used in each coin cell fabrication.

Electrochemical characterizations:

Cyclic voltammetry was performed using an Ametek potentiostat at a scan-rate of 0.1 mV/s with vertex potentials of 0.01 and 3 V. The galvanostatic charge discharge measurements were carried out with MTI corporation battery analyzer at variable current densities from 0.05 Ag^{-1} to 2 Ag^{-1}. The electrochemical impedance spectroscopy (EIS) measurements were studied using the Ametek potentiostat instrument within a frequency range of 300KHz to 100 mHz.

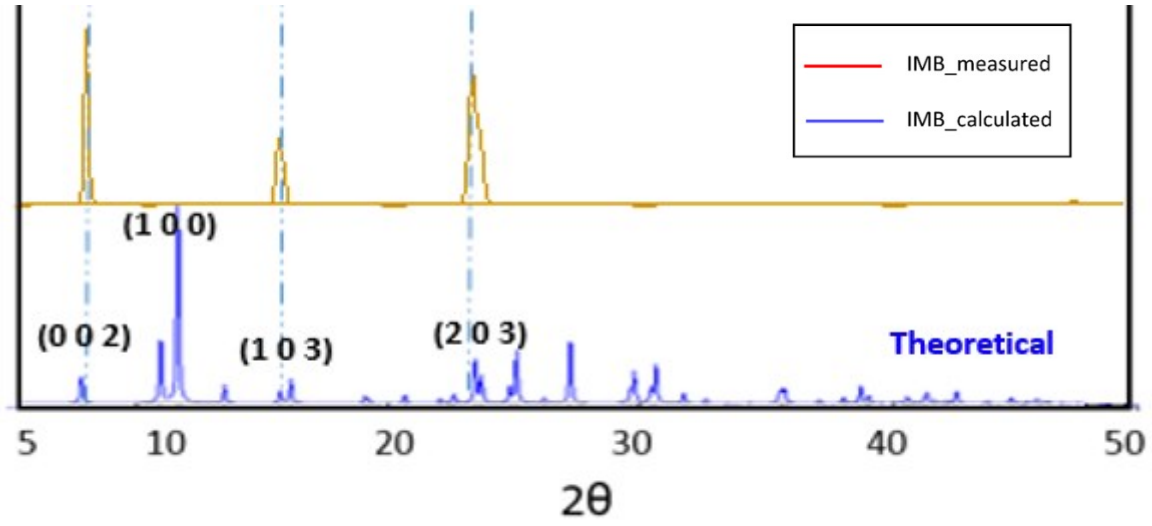


Fig S1. Powder XRD data of IMB (Simulated and experimental), with preferred orientation indicated

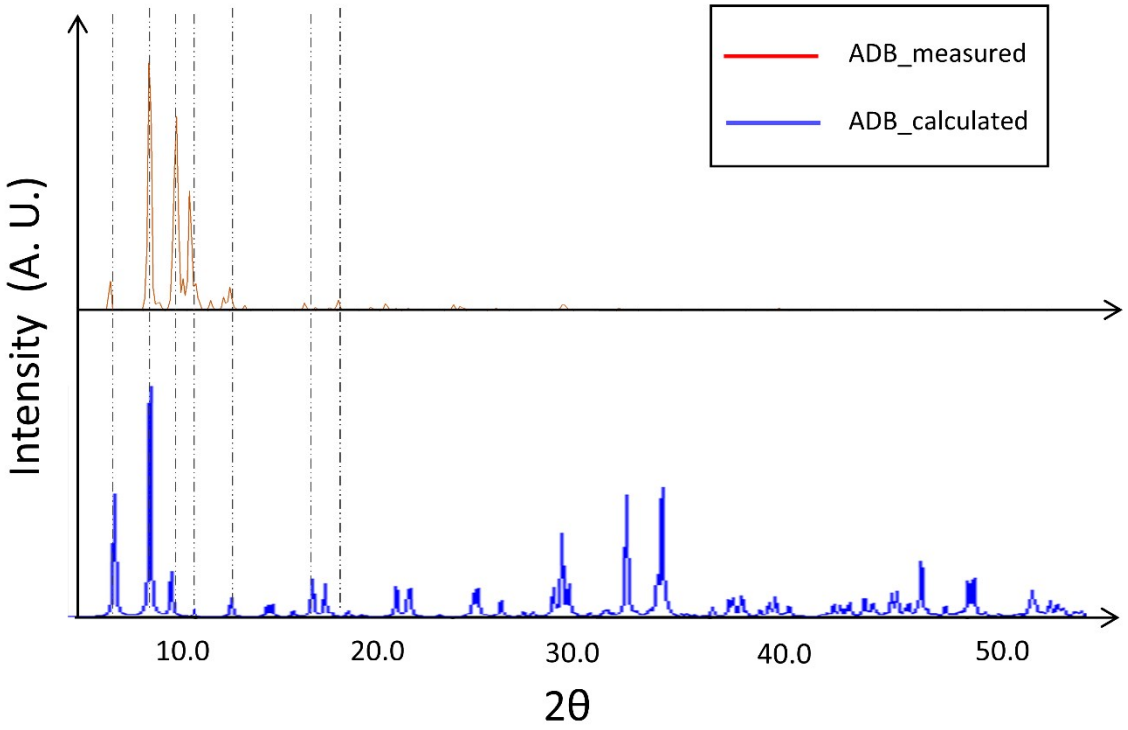


Fig S2. Powder XRD data of ADB (Simulated and experimental)

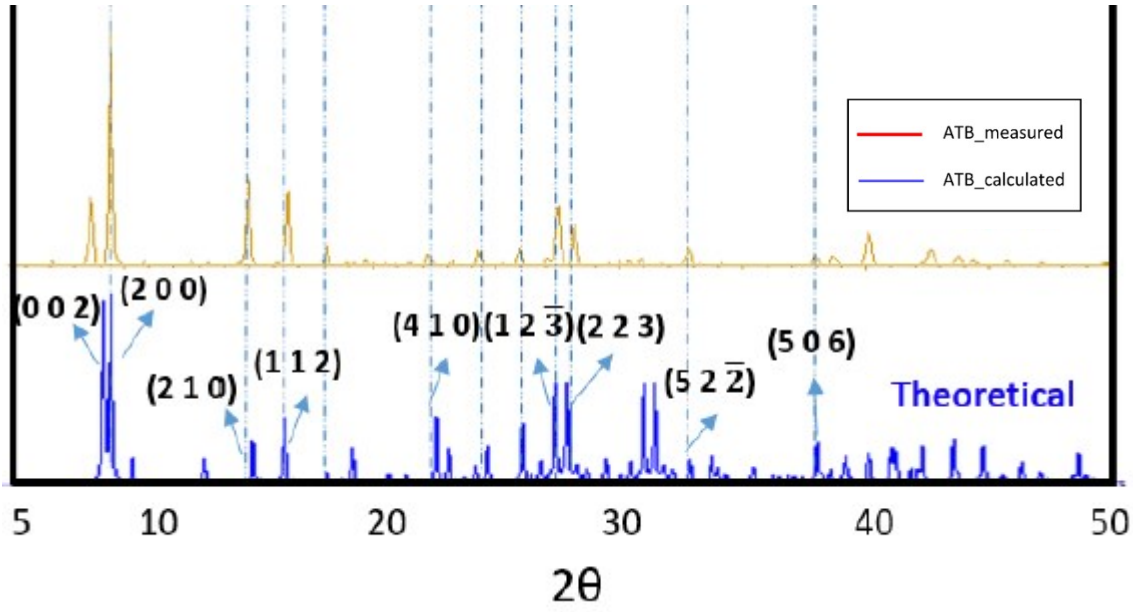


Fig S3. Powder XRD data of ATB (Simulated and experimental), with preferred orientation indicated.

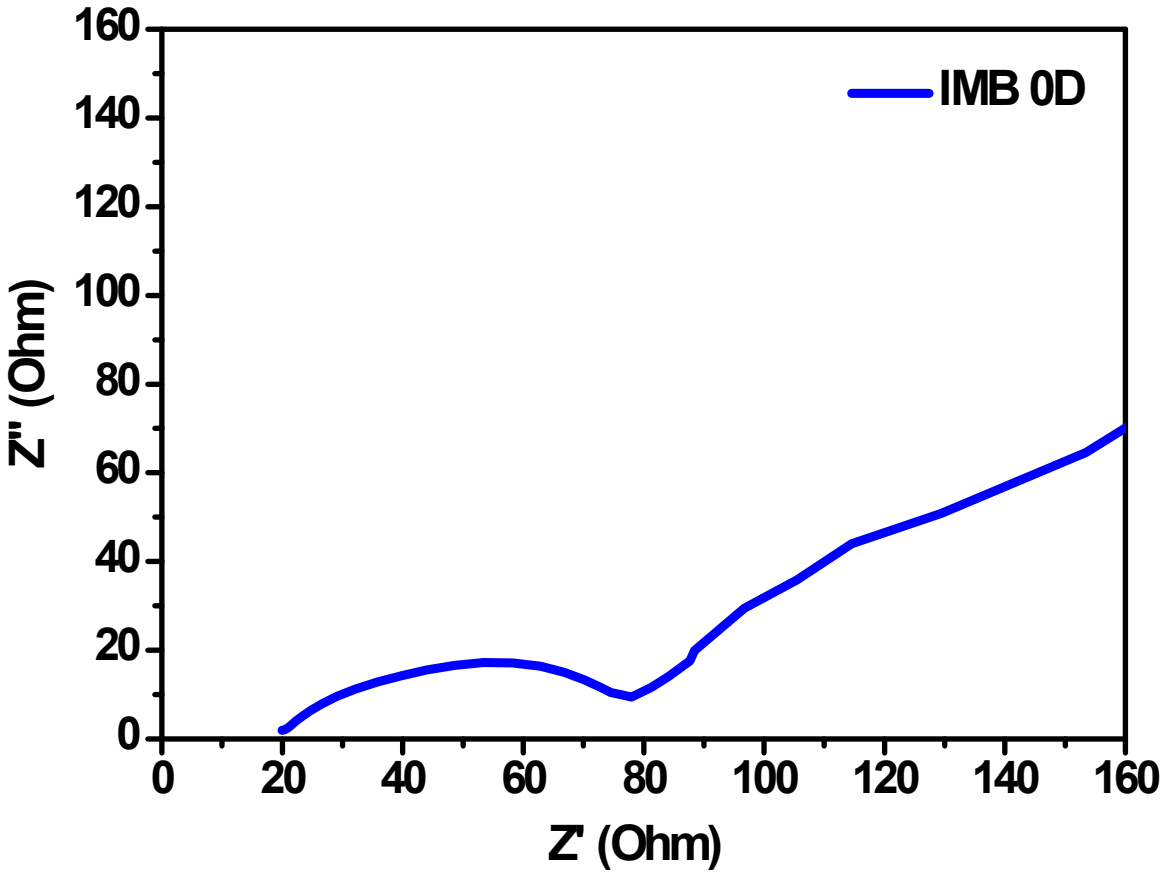


Fig S4. Electrochemical impedance spectra of the IMB cell. Frequency range: 300 KHz to 100 mHz

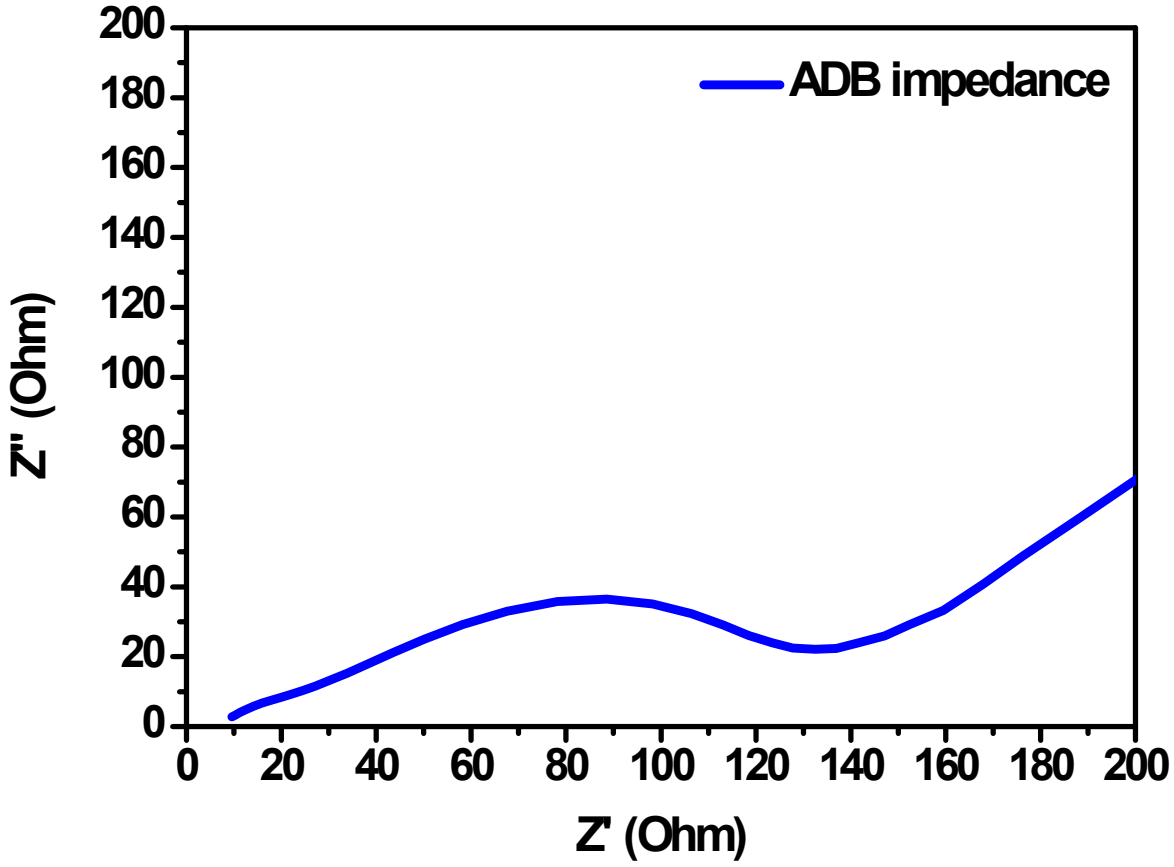


Fig S5. Electrochemical impedance spectra of the ADB cell. Frequency range: 300 KHz to 100 mHz

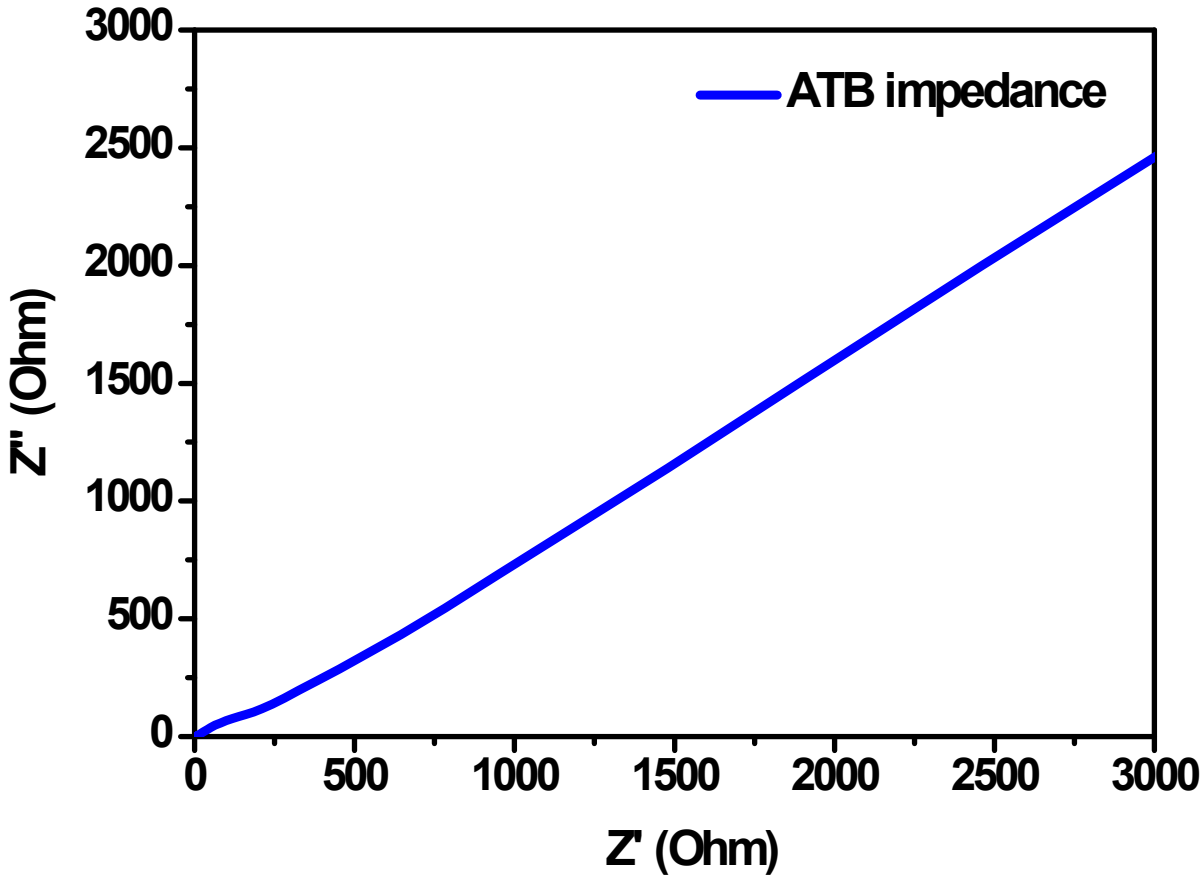


Fig S6. Electrochemical impedance spectra of the ATB cell. Frequency range: 300 KHz to 100 mHz

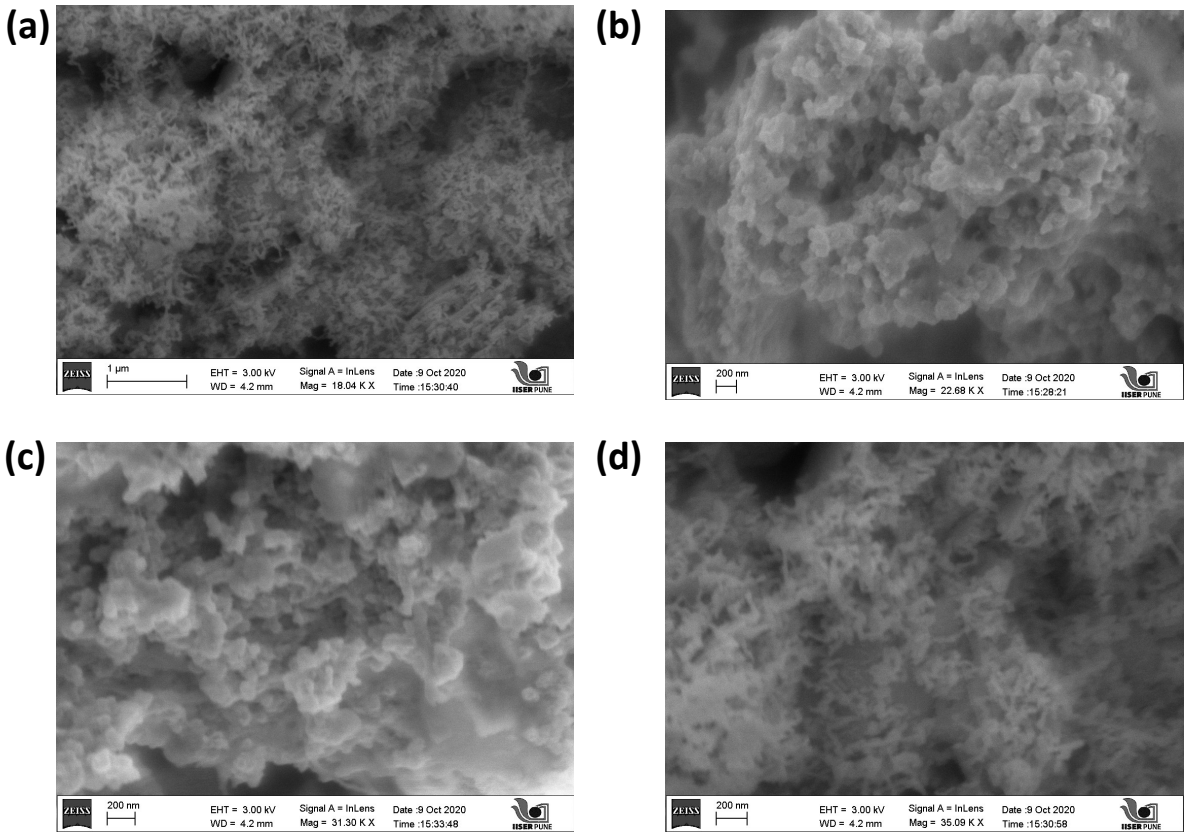


Fig S7. FESEM images of the IMB electrode.

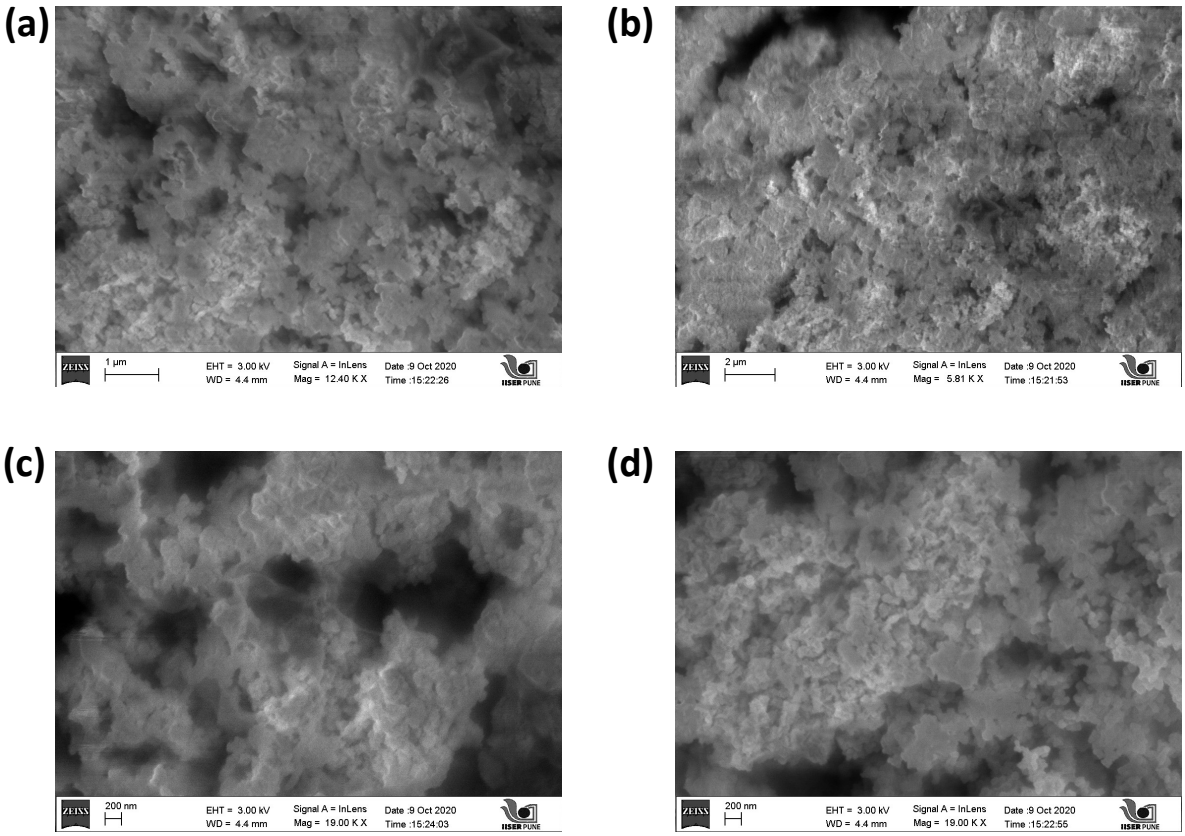


Fig S8. FESEM images of the ADB electrode.

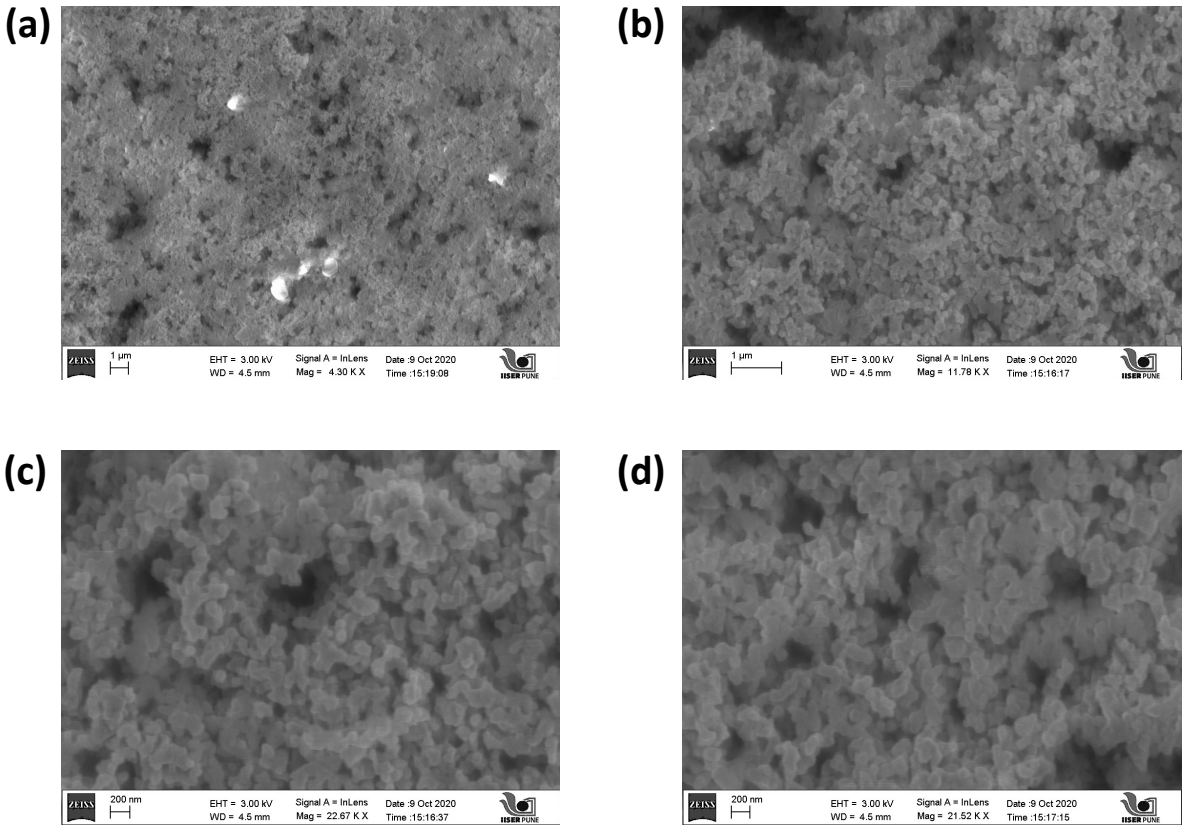
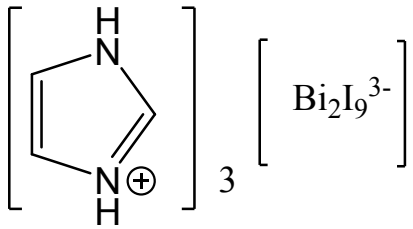
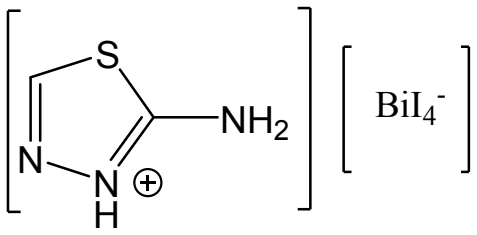


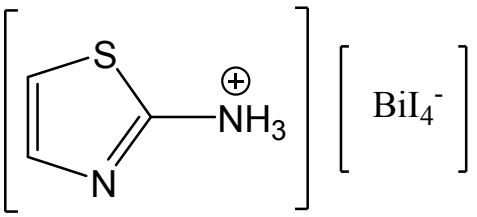
Fig S9. FESEM images of the ATB electrode.



Imidazolium bismuth iodide (IMB); $[C_3H_5N_2]_3[Bi_2I_9]$



2-amino-1,3,4-dithiazolium bismuth iodide (ADB); $[C_2H_4N_3S][BiI_4]$



2-aminothiazolium bismuth iodide (ATB); $[C_3H_5N_2S][BiI_4]$

Fig S10. Molecular structures of IMB, ADB and ATB.