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Lithium-ion batteries (LIBs) are well established energy storage devices for electronic, transportation and renewable-energy applications. Nevertheless, to meet the ever-increasing energy storage demand for electrical mobility and smart grid, future batteries have to guarantee higher energy density and, at the same time, sustainable and cheaper solutions. In this frame anode and cathode materials with higher specific capacity are required.

From the cathode side, according to preliminary DFT calculations, carbon nitride (g-C_3N_4) was selected and investigated as lithium polysulfides trapping agent in Li-S battery, using a double-layer approach. Carbon nitride was synthetized by a simple thermal condensation route using different precursors, with the aim of evaluating the polysulfides trapping ability in relation with morphology and surface chemistry of different g-C_3N_4 materials.

In a second step, g-C_3N_4 was synthetized from urea at different temperatures showing variations in specific surface area and surface functionalities. In particular, different amounts of pyridinic nitrogen, directly interacting with lithium polysulfides, were detected. In conclusion, carbon nitride obtained from urea at 550 °C resulted to be the best candidate as trapping agent in the double-layer sulphur cathode and the electrode containing carbon nitride demonstrated long cycling performances, for more than 500 cycles, as well as better electrochemical performances at higher C-rates.

Concerning the anode electrode, tin oxide-based materials were investigated. Two different strategies were presented in order to limit the rapid capacity fading of tin oxide anode, increasing the reversibility of the conversion reaction and at the same time containing the huge volume expansion. The first strategy was a simple and scalable wet impregnation synthesis, where tin oxide was directly grown on the surface of a commercial carbon black. The final hybrid compound, containing a particularly high amount of SnO_2 (30 wt.%), showed a specific capacity higher than 500 mAh g^{-1} for more than 500 cycles, with a coulombic efficiency of about 99.9 %. These outstanding electrochemical results were correlated to an optimal distribution of small tin oxide nanoparticles directly anchored to C45 surface.

The second strategy adopted g-C_3N_4, already used for the cathode material, as high surface support for tin dioxide growth. In this case, a simple solid-state synthesis was selected, and the SnO_2 precursors were directly mixed with carbon nitride. The final hybrid compound showed a final amount of SnO_2 of about 90 wt.% and a huge specific surface area able to contain the volume expansion of tin oxide particles during the alloying process. The final compound showed good electrochemical results, presenting a specific capacity of about 500 mAh g^{-1} for 100 cycles at 1C, and interesting results at higher current regimes.

Last but not least all the synthesis approaches studied in this work resulted valid strategies to increase the electrochemical performances while being simple, sustainable and easily up-scalable.

References

[1] Versaci et al. *Solid State Ion.* **2020,** 346, 115210
[2] Versaci et al. *Electrochim. Acta* **2021,** 367, 137489
[3] Versaci et al. *Appl. Mater. Today* **2021,** 25, 101169