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Improving the electrochemical properties of MXene Ti_3C_2 multilayer for Li-ion batteries by vacuum calcination

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Abstract: The electrochemical properties of MXene Ti_3C_2 multilayer for Li-ion batteries were improved greatly by vacuum calcination, after systematically evaluating its thermal stability in different atmosphere in details. In air, the as-prepared Ti_3C_2 could not be oxidized up to 429.9 ^oC and the rutile-TiO_2 would remain as the oxidation product at 1200 ^oC. The surface functional groups especially F groups can be eliminated by heat treatment. After vacuum calcination at 400 ^oC, the Ti_3C_2 show much higher capacities due to the removal of OH groups (126.4 $mAh \cdot g^{-1}$ at 1C), and exhibited excellent rate capability. Besides, the formation of TiO_2 nanoparticles at 700 ^oC further increases the first coulombic efficiency (62%) and capacity retention after 100 cycles (97%). In contrast, the dense microstructures of resulting TiC_x formed after calcination at 1000 ^oC results in the worst electrochemical properties. This paper presented a relatively simple and easily scalable post-treatment for improving the electrochemical properties of MXene, and demonstrated a great potential of Ti_3C_2 of using as anode material for Li-ion batteries.

Keywords: Thermal stability; Multilayer Ti_3C_2; Vacuum calcination; Electrochemical properties; Li-ion batteries

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