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1 Improving the electrochemical properties of MXene Ti₃C₂ multilayer

2 for Li-ion batteries by vacuum calcination

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Abstract: The electrochemical properties of MXene Ti_3C_2 multilayer for Li-ion 8 9 batteries were improved greatly by vacuum calcination, after systematically evaluating its thermal stability in different atmosphere in details. In air, the as-10 11 prepared Ti_3C_2 could not be oxidized up to 429.9 °C and the rutile-TiO₂ would remain 12 as the oxidation product at 1200 °C. The surface functional groups especially F groups can be eliminated by heat treatment. After vacuum calcination at 400 $^{\circ}$ C, the Ti₃C₂ 13 show much higher capacities due to the removal of OH groups (126.4 mAh \cdot g⁻¹ at 1C), 14 15 and exhibited excellent rate capability. Besides, the formation of TiO₂ nanoparticles at 700 °C further increases the first coulombic efficiency (62%) and capacity retention 16 after 100 cycles (97%). In contrast, the dense microstructures of resulting TiC_x 17 formed after calcination at 1000 °C results in the worst electrochemical properties. 18 19 This paper presented a relatively simple and easily scalable post-treatment for 20 improving the electrochemical properties of MXene, and demonstrated a great 21 potential of Ti₃C₂ of using as anode material for Li-ion batteries.

22 *Keywords*: Thermal stability; Multilayer Ti₃C₂; Vacuum calcination; Electrochemical

23 properties; Li-ion batteries

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