

Supporting information

***In-situ* grown Nb₄N₅ nanocrystal on nitrogen-doped graphene as a novel anode for lithium ion battery**

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Experimental section

Fabrication of graphene oxide (GO): 3 g graphite powder was added to 360 mL concentrated sulfuric acid and 40 mL phosphoric acid in an ice-bath with vigorously stirring for 30 min. Then, 18 g potassium permanganate was slowly added to the above solution and stirred for 1 h. Then, the mixture was maintained at 50 °C for 12 h. The resultant bright yellow suspension was poured into a 1000 mL flask contained 400 g ice, following by adding 3 mL H₂O₂ solution which reduces residual MnO₄⁻ to Mn²⁺. The precipitate was transferred into dialysis and carried out by dialysing in DI water in order to remove the residual Na⁺, K⁺, SO₄²⁻ and other ions. Last, the precipitation was treated by vacuum drying for 48 h.

TG-DSC analysis

The initial weight of sample is 5.3724 mg and the last weight is 5.3817 mg. We assume that the the weight of Nb₄N₅ is x mg and the N-G is y mg. So $x + y = 5.3724$ mg. From ca. 150 to ca. 400 °C, the weight increases because the 1 molecular Nb₄N₅ is oxidated to be 2 molecular Nb₂O₅. The weight decreases from ca. 400 to ca.800 °C due to the combustion of N-G and the oxidation of Nb₄N₅. The molecular weight of Nb₄N₅ is 441.6592 g mol⁻¹ and the molecular weight of Nb₂O₅ is 265.8098 g mol⁻¹. The oxidation of Nb₄N₅ can lead that the weight (except N-G) increases to be 1.2037 x mg (Nb₂O₅). Around 800 °C, the combustion finish and the oxidation complete. The result indicates that 1.2037 $x = 5.3817$ mg. So $x = 4.4710$ mg and $y = 0.9014$ mg. The content of N-G in Nb₄N₅/N-G is about 16.78 %.

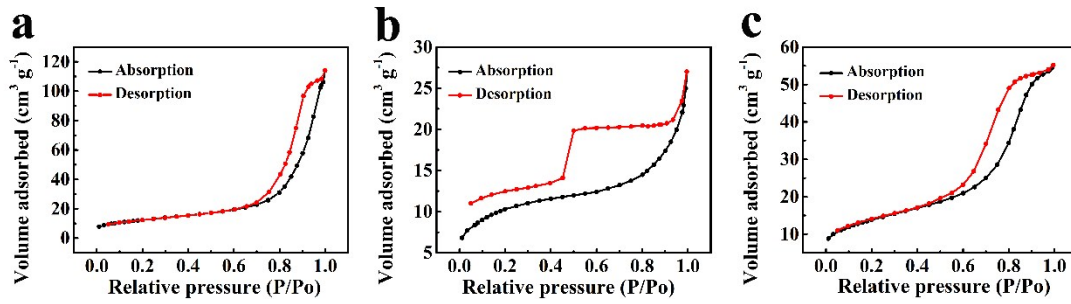


Figure S1. N₂ sorption isotherm of (a) bare Nb₄N₅, (b) N-G and (c) Nb₄N₅/N-G.

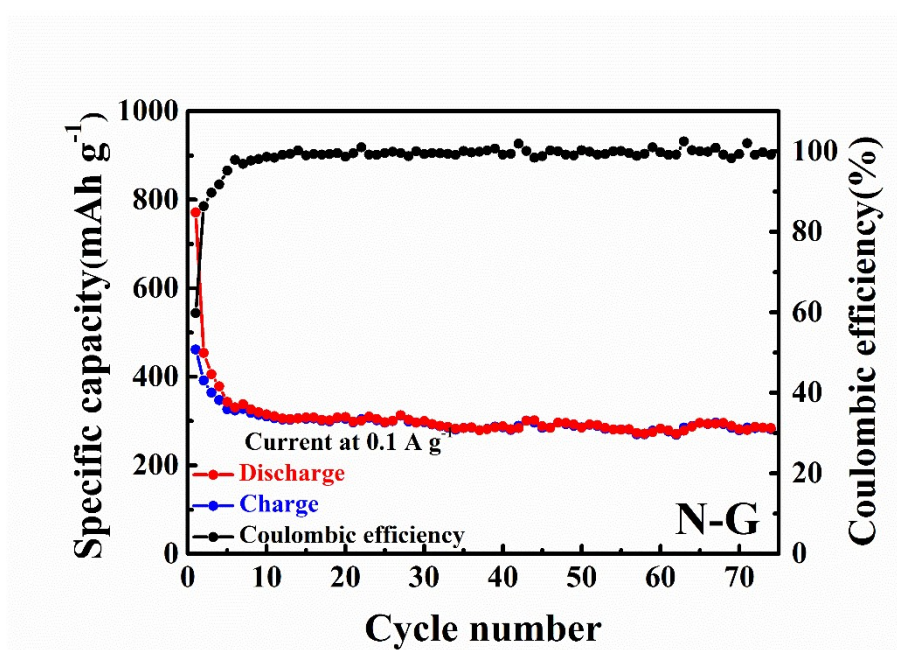


Figure S2. Cycle performance and coulombic efficiency of N-G at 0.1 A g⁻¹ (0.0832 mA cm⁻²).