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MXene Quantum Dots Decorated Double-Shelled Ceo₂ Hollow Spheres for Efficient Electrocatalytic Nitrogen Oxidation

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Abstract : Direct electrocatalytic nitrogen oxidation (NOR) provides a promising alternative strategy for synthesizing high-value-added nitric acid from widespread N_2, which overcomes the disadvantages of the Haber-Bosch-Ostwald process. However, the NOR process suffers from the limitation of high N≡N bonding energy (941 kJ mol− ¹), sluggish kinetics, low efficiency and yield. It is a prerequisite to develop more efficient electrocatalysts for NOR. Herein, we synthesized double-shelled CeO_2 hollow spheres (D-CeO_2) and further modified with Ti_3C_2 MXene quantum dots (MQDs) for electrocatalytic N_2 oxidation, which exhibited a NO_3− yield of 71.25 μg h− ¹ mgcat− ¹ and FE of 31.80% at 1.7 V. The unique quantum size effect and abundant edge active sites lead to a more effective capture of nitrogen. Moreover, the double-shelled hollow structure is favorable for N_2 fixation and gathers intermediate products in the interlayer of the core-shell. The in-situ infrared Fourier transform spectroscopy confirmed the formation of *NO and NO_3− species during the NOR reaction, and the kinetics and possible pathways of NOR were calculated by density functional theory (DFT). In addition, a Zn-N_2 reaction device was assembled with D-CeO_2/MQDs as anode and Zn plate as cathode, obtaining an extremely high NO_3− yield of 104.57 μg h− ¹ mgcat− ¹ at 1 mA cm− ².

Keywords : electrocatalytic N_2 oxidation, nitrate production, CeO_2, MXene quantum dots, double-shelled hollow spheres
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