World Academy of Science, Engineering and Technology International Journal of Materials and Metallurgical Engineering Vol:18, No:05, 2024

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

Authors : Quan Li, Dongcai Shen, Zhengting Xiao, Xin Liu Mingrui Wu, Licheng Liu, Qin Li, Xianguo Li, Wentai Wang **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 $N \equiv N$ 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 μ g 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 $104.57 \mu g h-{}^1$ mgcat $-{}^1$ at 1 mA cm $-{}^2$.

Keywords: electrocatalytic N2 oxidation, nitrate production, CeO2, MXene quantum dots, double-shelled hollow spheres

Conference Title: ICMSE 2024: International Conference on Materials Science and Engineering

Conference Location : Sydney, Australia **Conference Dates :** May 16-17, 2024