Highly Active and Stable Nickel-Molybdenum Nitride (Ni_2Mo_3N) Electrocatalysts for Hydrogen Evolution

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Transition metal nitrides (TMNs) are promising HER catalysts owing to the high electrical conductivity, corrosion resistance, and similar electronic structures to Pt. However, since the monometallic TMNs still showed inferior activity than Pt-based catalysts, bimetallic TMNs have been studied to improve HER activity. The presence of a second metal atom in bimetallic TMNs could provide more reaction sites and improve electronic conductivity compared to monometallic TMNs. Especially, nickel molybdenum nitride (Ni-Mo-N) are known as representative bimetallic TMNs with high HER activity.

Herein, we easily fabricated bimetallic Ni_2Mo_3N on Ni foam by simple annealing of Mo precursor and Ni foam in one-pot. In synthesis, Ni foam acted as Ni precursor because Ni atoms are released from the Ni foam during annealing and toxic NH_3 gas was not used. The resultant nanosized Ni_2Mo_3N/NF (ca. 7 nm) showed noticeably outstanding HER activity with low overpotential (η_{10} = 21.3 mV) and excellent stability for 24 h. In addition, our DFT calculation suggested that structural characteristics of the N active sites affect the HER activity.