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Electrochemically formed Single-Atom Centers of MXenes for the Selective Electrochemical Reduction of Nitrogen to Ammonia

The electrochemical nitrogen reduction reaction (NRR) presents a sustainable route for ammonia production under ambient conditions. MXenes, with their unique physicochemical properties, have shown promise as electrocatalysts for NRR. However, the competitive hydrogen evolution reaction (HER) limits their selectivity. Here, we propose a strategy leveraging the in-situ electrochemical formation of single-atom catalyst (SAC)-like centers on MXenes under anodic polarization, combined with cathodic potential pulses to activate nitrogen reduction at these SAC sites. The DFT calculations reveal that such dynamically formed MXene-SAC sites suppress HER and enhance NRR activity by tuning adsorption energies and electronic properties. This work opens pathways to design potential electrocatalysts for sustainable ammonia synthesis.

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