Revealing the Unique Catalytic Landscape of Anti-MXene Borides for Nitrogen and Nitrate Reduction

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Two-dimensional anti-MXene borides (TMBs) represent a groundbreaking class of materials offering exceptional catalytic potential for nitrogen reduction (NRR) and nitrate reduction reactions (NO3RR). This study delves into their catalytic mechanisms using state-of-the-art density functional theory (DFT) calculations. Key findings highlight FeB and OsB as top-performing catalysts in the NRR, showcasing low limiting potentials and suppression of competing hydrogen evolution reactions. Meanwhile, MnB, RhB, and IrB exhibit diverse NO3RR pathways, selectively converting nitrate to ammonia or nitrogen gas. Comprehensive analyses of stability, electronic structure, and adsorption energetics confirm the catalytic versatility of these materials, opening pathways for environmental applications in sustainable ammonia production and water remediation. This research establishes anti-MXene borides as promising candidates for electrocatalysis, addressing pressing global energy and environmental challenges.

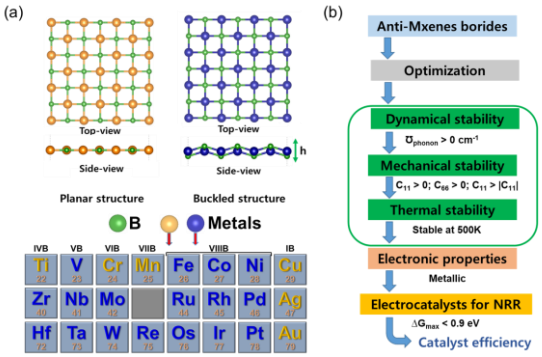

Figure 1. Illustration and criteria for anti-MXene borides as NRR (or NO3RR) electrocatalysts