Electrochemical generation of ammonia using MXenes

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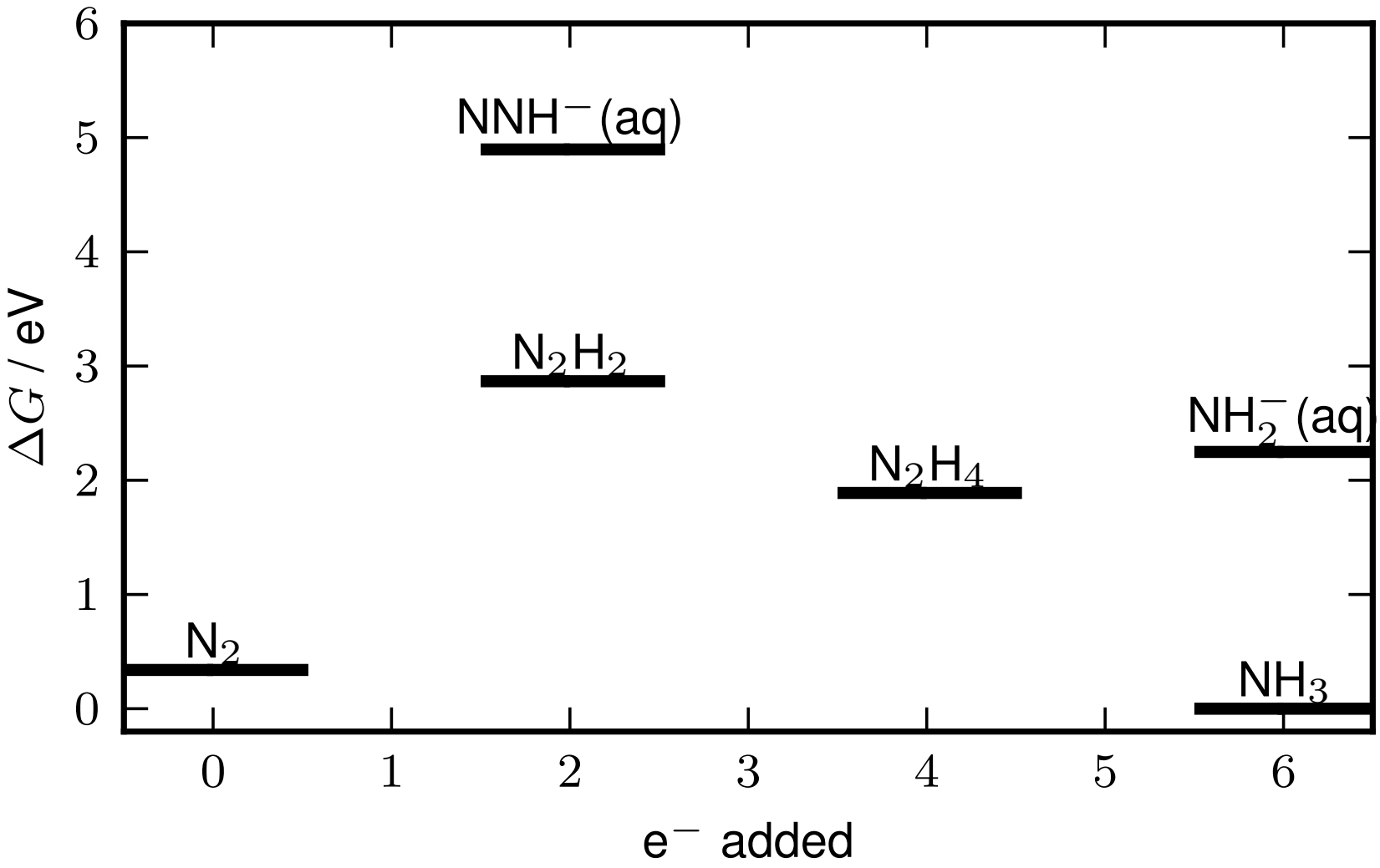
Electrifying Everything

RE2X: Electrosynthesis

Ammonia: 0.5
Gtons

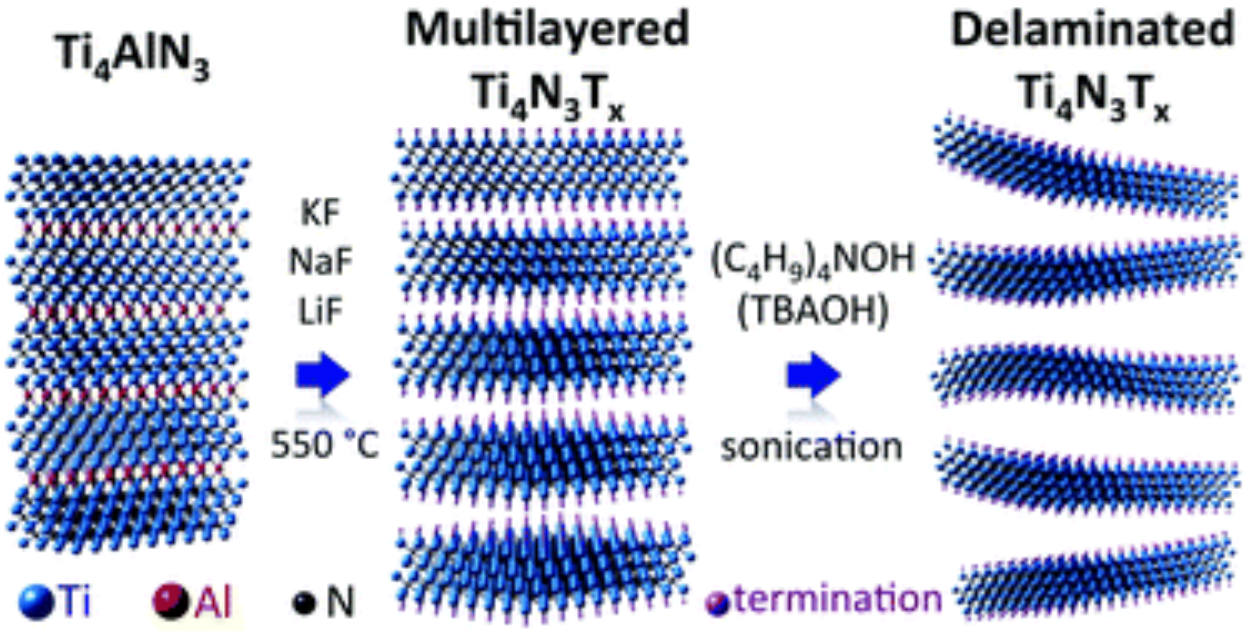
Typical Free Energy Landscape



Mxene Nitrides

Etching can leave surface terminations that provides tunability

- F
- O
- OH

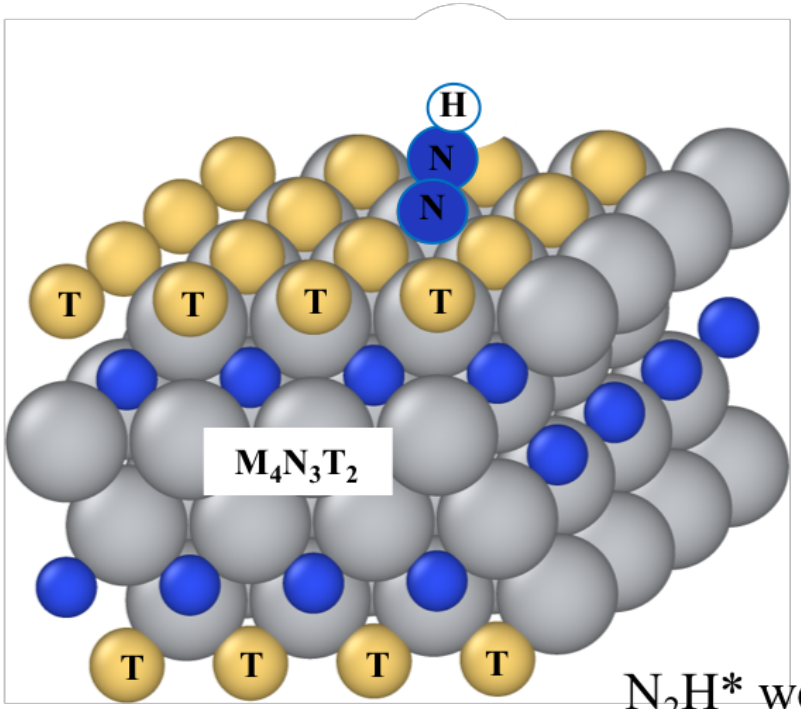


Urbankowski, *et al*, *Nanoscale* (2016) 8, 11385-11391
Urbankowski, *et al*, Nanoscale (2017) 9, 17722-17730

Formation Energy

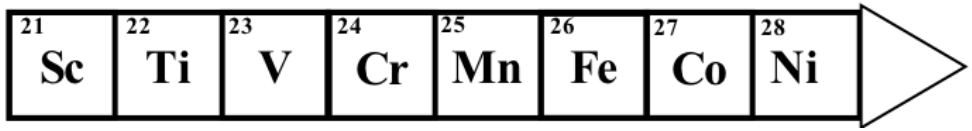
Termination	$Ti_4N_3T_2$ [eV]	$Sc_4N_3T_2$ [eV]
Non-terminated	-2.17 (AA)	-2.56 (AA)
F	-5.47 (AA)	-6.54 (AA)
O	-5.76 (AA)	-5.56 (AA)
OH	-5.37 (AB)	-6.28 (AA)

Design Principles for Broader Screening



- OH-terminated MXenes bind without dissociation;
- Non-terminated, low termination coverage, O-, and OH-terminations trigger dissociative pathways.
- F-termination has HF formation tendency
- Explore mixed MXenes and propose other etching agents

N_2H^* weakening



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Thank you