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Electrocatalysis of Nitrogen-Based Fuels: Fundamental Questions and Complex Materials

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Storing energy in the nitrogen cycle ($N_2 \rightleftharpoons$ N-based fuel) is a promising, yet thorny route, towards energy sustainability. The nitrogen cycle is even harder to tame than the much investigated and still baffling hydrogen/oxygen cycle ($H_2O \rightleftharpoons H_2$ fuel). Featuring a broad range of oxidation states, and multiple stable intermediates, the nitrogen cycle is a rich and daunting challenge for electrocatalysis.

Complex multi-doped carbons are promising catalysts in the nitrogen cycles, yet their composition – not to mention catalytic site identification – is still uncertain. Materials such as Fe–N–C can oxidize hydrazine fuel and reduce N_2 and NO_x compounds, through a range of atomic, molecular, and nanometric catalytic sites. Understanding these is the key to the development of sustainable and platinum-free electrocatalysts.

My group aims to unravel the complex structure and activity of such materials, in order to design new reactivity in the nitrogen cycle. Focusing on hydrazine, urea and ammonia fuels, our dream is to identify active sites, reaction mechanisms, and selectivity controls. Among our surprising discoveries are the true role of doping cooperativity in multi-doped carbons, the unique mechanism by which pore size determines reaction selectivity, and the unexpectedly detrimental role of Fe_3C, a commonly lauded component of most Fe–N–C materials. These findings help us develop new, active and stable catalysts for direct nitrogen-fuel fuel cells.

(some recent references: Ojha *et al.*, *Angew. Chem. Int. Ed.* **2018**, *57*, 17168; Burshtein et al., *J. Mater. Chem. A* **2019**, *7*, 23854; Burshtein *et al.*, *Phys. Chem. Chem. Phys.* **2021**, *23*, 26674; Farber *et al.*, *J. Mater. Chem. A* **2022**, *in print*)