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תוכנית האנרגיה ע"ש גרנד

The Laboratory for Organic and Inorganic Chemistry

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Earth-Abundant Electrocatalysts for the Nitrogen Cycle

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Electrocatalysis in the nitrogen cycle involves many aspects of our lives, from environmental and industrial processes to the energy sector. Ammonia (NH_3) is commonly used for nitrogen-based fertilizers, crucial for agriculture. Consequently, ammonia, along with urea ($CONH_2$) are polluting our ground water and wastewater, which calls for water remediation by oxidation to nitrogen. Moreover, Ammonia and urea have been recently gaining attention by the energy sector as possible hydrogen carriers, or as nitrogen-based fuels for direct fuel cell applications. Hydroxylamine (NH_2OH) is an intermediate in the nitrogen cycle with a key role in these reactions. Hydrazine is another nitrogen-based fuel alternative, with a very high energy density and the highest theoretical cell voltage of all liquid fuels. Largely, nitrogen-based fuels cells do not involve CO_2 emissions, with the added advantage of easier and safer handling of the fuel than hydrogen.

The electro-oxidation of these molecules requires an electrocatalyst, to reduce the activation energy and to allow higher outputs. Specifically, affordable and abundant materials should be considered for a wide-spread commercial application. In this research, the relationship between the nature of the active site structure and the resulting electrocatalytic activity will be investigated for Ni and Fe-N-C based low-cost catalysts, in the nitrogen cycle.

Nickel hydroxide is a prominent catalyst in many of these nitrogen cycle reactions in the form of its oxidized phase, nickel oxyhydroxide (NiOOH), tying the $Ni^{II} \rightarrow Ni^{III}$ transition to any electrocatalytic reaction. However, the $Ni(OH)_2$/NiOOH transitions entail complicated innate electrochemistry involving different phase transformations. Despite over a century of Ni electrochemistry, the effects of the crystallographic phase and phase transitions on the activity are still not fully understood. A systematic analysis of the connection between the nickel hydroxide phases and crystalline disorder with its behavior towards urea and ammonia oxidation will be presented. Furthermore, iron and nitrogen doped carbons (Fe-N-Cs), with single atom Fe sites, have emerged as outstanding non-PGM catalysts for some fuel cell reactions. They are versatile and include highly abundant materials. However, the nature of the FeN4 active site is still not elucidated. Herein, Fe-N-C catalysts are evaluated for hydroxylamine and hydrazine oxidation, providing insight on the nature of the active site and the resulting activity. Consequently, we designed an open and accessible active site, achieving a record-breaking direct hydrazine fuel cell performance based on Fe-N-Cs. This research emphasizes the importance of understanding the catalyst structure for a rational design of catalysts for nitrogen-based fuel cells towards improved activity for energy applications.