



Applications of the Carbon in Metal-Based Electro Catalysts towards Green Nitrogen Fixation

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DESCRIPTION

Electrochemical conversion of molecular nitrogen to high-value ammonia products is an interesting strategy to meet the growing global demand for a wide range of applications, from agricultural fertilizers to advanced areas of energy storage. To date, the Haber-Bosch process remains one of the most important leaps in industrial chemistry and the power society during the industrial revolution. In fact, when assessing the environmental impact of this reaction, we need not just focus on the energy required to maintain the high temperature and pressure. In fact, the hydrogen used in this process historically comes from Steam Reforming (SMR) and Water Gas Shift Reaction (WGSR). Today, the ammonia synthesis process accounts for more than 1% of the world's energy demand, and research has since followed various strategies based on low-pressure and low-temperature processes, hybrid designs combining the electrochemical generation of hydrogen with the Haber-Bosch process, and finally focused. Electrochemical Nitrogen Reduction Reaction have the growing interest in NRR catalysts capable of high selectivity (i.e., able to suppress the Hydrogen Evolution Reaction (HER) at the cathode), carbon-based electrodes gained attention towards its low cost and versatility. They act as an active catalyst and as a support. In particular stabilization of the active site is of paramount importance in these types of materials given the reliance on intrinsically unstable structures leads to defect sites, unusual facets or single-atom catalysts. A vast number of studies have been carried out centered on this key topic, ranging from the more classical approach of N- or B-monodoped porous carbon materials to the more complex co-doping heteroatom strategy and furthermore to tunable edge sites and topological intrinsic defects in the carbon matrix.

Aqueous environment (that includes acidic, basic or neutral solutions) represents the most widely adopted electrolyte that exploits the H⁺ or OH⁻ charge carriers. Stable materials in this reaction media comprise many types of different N₂ electro catalysts, including transition metal-based materials (alloys, nitrides, sulfides, oxides, etc.), but also other classes, including

heteroatom-doped metal-free carbon textures and Single-Atom Catalysts (SACs) are generally doped carbon functions as support for the single-metal site. Adequate surface area and porous structure, and appropriate defect formation to facilitate N₂ adsorption and conversion. Therefore, heteroatom-doped (usually nitrogen or boron) carbon-based nanostructures may be a promising strategy to improve NRR given the wide range of existing CNSs.

Not only common Carbon Nanotubes (CNTs), Carbon Nanohorns (CNHs), graphene and related structures, but also more advanced materials such as Carbon Dots (CDs) exhibit high electrochemical solubility in many solvents, large ratios. It belongs by basic characteristics such as surface area and relevance. Inexpensive features that can be modified with edge sites for functionalization, attractive surface chemistries and other modifiers/nanomaterials.

On the other side, it is important to highlight the N-doped carbon catalysts which could be subjected to degradation during the process by releasing ammonia into the electrolysis solution as an external source and they are not directly arising from NRR, affecting true activity evaluation. In consideration of all the other numerous difficulties in rigorously evaluating the activity of NRR catalysts, it is critical to perform required additional measurements or have precise control of experimental parameters. Nevertheless, N-doped carbon-based catalysts still represent one of the most investigated strategies includes a porous carbon material prepared by ZIF-8 treatment and the N-doped carbon nano spikes designed by using numerous graphene-based structures. Considering graphene as a representative study it has been demonstrated by several other studies for the general requirement to enhance the catalytic performance to endow adequate charge carrier mobility is to promote a charge transfer during NRR combined with a structural stability. Many different theoretical studies on NRR (and also on other electrochemical reduction processes) have indeed focused on graphene as the nano carbon phase, in particular for the class of SAC electro catalysts.

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