

# Engineering Electrical Structure to Accelerate the Oxygen Evolution Reaction on Graphene

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## Editorial

A water-splitting electro catalyst that is effective, stable under working conditions, and made of materials that are abundant on Earth would make it easier to realise a hydrogen economy. With a single-walled carbon nanotube serving as a model catalyst, density functional theory simulations of the more challenging half-reaction, the anodic oxygen evolution reaction, reveal that nitrogen dramatically lowers the necessary over potential in comparison to the pristine nanotube [1]. The systems and active sites with different nitrogen functionalities, such as graphitic, pyridine, or pyrrole, which were produced by adding nitrogen and basic lattice flaws including atomic substitutions, vacancies, or Stone Wales rotations.

There are several nitrogen functions. The scaling relation predicted similar low over potentials near the summit of the volcano, which were closely observed by the graphitic, oxidised pyridine, and Stone Wales pyrrole nitrogen systems. The four-step single-site water nucleophilic attack mechanism was the OER mechanism taken into account. The creation of attached or peroxide moieties, which occurred in the second or third step in active systems, determined the reaction's potential [2]. By looking at similar graphene-based model systems, the impacts of nanotube radius and chirality were studied up to the limit of large radius. While they exhibited patterns resembling those of nanotube-based systems, they frequently had decreased reactivity as a result of the intermediate moieties' poorer adhesion. Renewable energy sources must have a scalable energy storage system due to their frequently erratic nature. This job can be filled by hydrogen produced by electrolytic water splitting. Therefore, effective electrolyzers hold the potential of a clean and sustainable global energy infrastructure, together with fuel cells and metal-air batteries. While the oxygen evolution reaction at the anode is sluggish as a result of the necessary four-electron transfer, the hydrogen evolution reaction at the electrolyser cathode is a two-step, two-electron process that is rather simple.

All four reaction steps would be equal and the kinetic barriers for the perfect catalyst would be vanishingly small, necessitating the use of an external voltage. However, in reality, even the greatest catalysts need a significant over potential, which wastes energy. A suitable rate of reaction, indicated by a current density, generated at a not very excessive over potential and a not too huge Tazal slope, which quantifies the needed over potential rise per decade increase in current density, is a useful indicator of catalyst efficiency. Only earth-abundant materials, durability under operating circumstances, and ease of fabrication are further prerequisites for a broadly applicable electro catalyst. As a result, extensive research is still being done to create electro catalysts that may satisfy these requirements [3]. The usage of precious metals as catalyst materials must be removed or drastically reduced for a hydrogen economy to be widely adopted. Alternative catalysts include non-precious metals. A thin

layer of the oxide or an oxide nanocluster placed on a conducting support can be used to improve the oxide material's frequently weak conductivity. Carbon nanotubes and graphene, which are Nano carbon materials, have a high conductivity, making them excellent supports

Alternately, Nano carbon systems without any metals, such as graphitic carbon nitride or their blends, may be used to make electro catalysts. Because pure and is comparatively inert, doping or cooping has been seen to enhance catalytic performance. The sidewall of the can be chemically functionalized with organic or organometallic chemical groups as an alternative to doping. Examined are the effects of the support material and the geometry that is important for material flows. The results are comparable to and occasionally even better than the best precious metal and transition metal oxide catalysts in terms of low over potentials and low Tazal slopes [4].

We have thoroughly examined active systems with different nitrogen doping functions, graphitic, pyridine, or pyrrole and defect architectures using the thermodynamic model in conjunction with attachment energies of intermediates. The activity of the initially rather inactive pure carbon systems significantly increased after the addition of nitrogen, often in conjunction with simple defects like vacancies and Stone Wales rotations. While the pristine system produced a predicted over potential, the same system doped with a single graphitic nitrogen atom produced a nearest neighbour activated carbon atom with a predicted over potential of with oxygen, via oxidation of a pyridine nitrogen. The Stone Wales system with a pyrrole nitrogen atom also produced good results [5]. The outcomes from the graphene-based systems were comparable, albeit frequently not much better. Additionally, we confirmed that the four-step single site method was appropriate for simulating OER on these systems, with the second or third phase formation of often serving as the crucial decision-making step.

The preliminary screening results of this study, along with our companion study of kinetic barriers on doped with inclusion of explicit solvent, demonstrate that inclusion of explicit solvent does not qualitatively change the thermodynamics mechanism, structures and attachment energies of intermediates, potential-determining step, or active site, despite being necessary for determining kinetic barriers. The effective over potentials, which include the kinetic barriers, may change, and the kinetic barriers in systems catalytic sites where thermodynamics analysis predicts similar activity and over potentials may occasionally.

## Conflict of Interest

None.

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