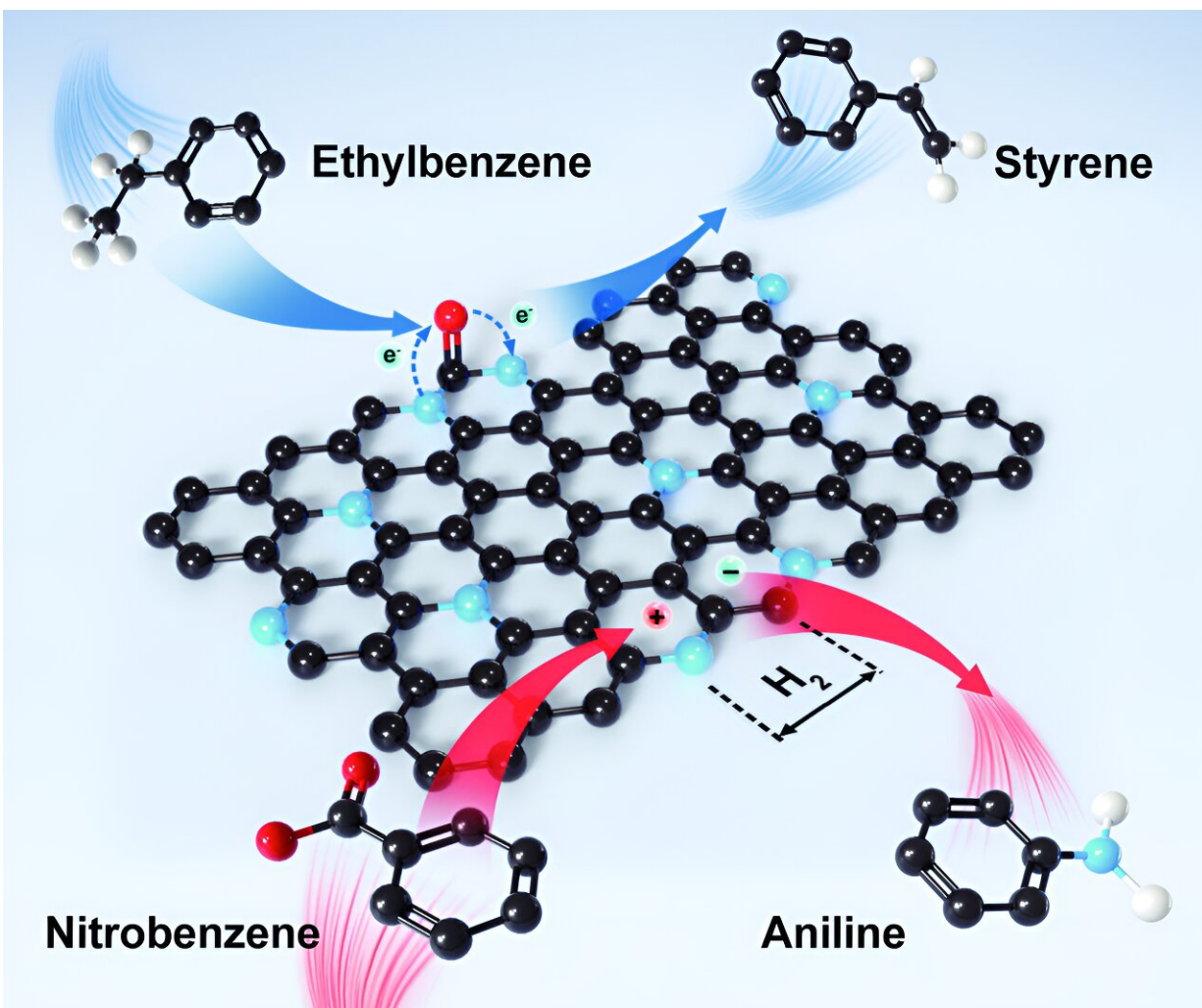


Guanine synthesis yields new insights into nitrogen's role in nanocarbon catalysis

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Scientists from Fuzhou University obtained a set of nanocarbons through self-assembling guanine molecules. Besides exhibiting intriguing properties, including relatively stable surface oxygen groups and high nitrogen content, the presence of multiple hydrogen bonds in guanine enabled the formation of a two-

dimensional nanosheet with controllable types of nitrogen dopants. The nitrogen content can be finely tuned from approximately 5 to 30 percent, while the oxygen content is kept at a consistent 4 percent. Credit: Zailai Xie; Fuzhou University

Recently, carbon-based catalysts—especially nitrogen-doped nanocarbons—have emerged as sustainable, reliable alternatives to the metal catalysts traditionally used to support chemical reactions.

Researchers from the Key Laboratory of Advanced Carbon-Based Functional Materials (Fujian Province University) at Fuzhou University synthesized nanocarbons from [guanine](#) molecules to better understand the precise role nitrogen plays in carbon-based materials and explore the reaction mechanisms of these catalytic systems.

In a recently published study, the research team clarified how different types of nitrogen can modulate oxidative dehydrogenation activity—a critical process involved in converting inert compounds into reactive nanocarbon.

The study was published in the journal [Carbon Future](#) on February 4.

"The study offers theoretical guidance for creating highly effective carbon catalysts, which could advance clean energies converted from [renewable resources](#) in industries like plastics, medicine and rubber," said study author Zailai Xie from Fuzhou University.

Doping carbon materials with heteroatoms such as nitrogen can change the carbon's properties. This practice has gained significant interest, driving researchers to investigate possible benefits. Nitrogen doping, in particular, has been shown to be a highly effective strategy in creating

[advanced materials](#) for carbon-dioxide capture, energy conversion, energy storage and other applications.

Despite the strides being taken in the field of nitrogen-doping, there are still some key questions that remain unanswered. For instance, the performance of nanocarbon materials is significantly influenced by functional groups of atoms on the surface—but, so far, nanocarbon materials exhibit uncontrollable surface functional groups, which complicates the identification of active sites for different types of reactions.

"This behavior hinders our understanding of the intrinsic role that nitrogen dopants play in improving [catalytic activity](#) and determining the catalytic mechanism," Xie said.

According to Xie, to further advance the field of nitrogen-doped nanocarbon catalysis, researchers need more controlled and better-characterized catalysts. This would allow researchers to isolate the effects of specific nitrogen species on catalytic performance.

In pursuit of this goal, the Fuzhou University research team developed a method to precisely control surface [functional groups](#), mainly oxygen and nitrogen groups, during nanocarbon catalyst generation.

The team obtained a set of nanocarbons through self-assembling guanine molecules—a compound found in guano or fish scales—and exposed the resulting material to heat without oxygen. Drawing inspiration from the supramolecular self-assembly of biological components like guanine and related nucleobases such as guanosine, this synthetic approach offers an intriguing means of generating ordered nanomaterials.

These molecules possess π -stacked, H-bonded, and other multiplex binding sites that facilitate the formation of functional supramolecular

assemblies. Guanine, being widely present in the biogenic photonic structures of various living organisms, exhibits diverse shapes and sizes, including hexagonal plates, square plates, irregular polygons, and prisms.

The subtle variations in the morphology of guanine crystals contribute to the colorful optical phenomena observed in animals, such as fish scales, spider bodies, and animal eyes. However, the precise control of the morphology of biogenic guanine crystals in organisms remains poorly understood.

Despite the remarkable properties of guanine crystals, the artificial production of regular guanine crystals that closely mimic biological conditions and their subsequent transformation into functional carbon materials has not yet been achieved in the chemical synthesis approach.

"The synthesized carbons exhibited unique and intriguing properties, including relatively stable surface oxygen groups and high nitrogen content," Xie said.

In addition, the presence of multiple hydrogen bonds in guanine enabled the formation of a two-dimensional nanosheet with controllable types of nitrogen dopants. The nitrogen content can be finely tuned from approximately 5% to 30 at%, while the oxygen content can be kept at a consistent 4%.

"This unique property makes guanine an ideal proof-of-concept precursor for construction model catalysts that can lead to in-depth understanding of the role of high nitrogen dopants in nanocarbon catalysis," Xie said.

To further probe the structure-function relationships, the team tested dehydrogenation and hydrogenation reactions, in which hydrogen molecules are stripped off or added to a larger molecule. The tests

demonstrated that different types of nitrogen in the nanocarbons, namely graphitic nitrogen and pyridinic nitrogen, serve as electron-donating and electron-withdrawing modulators, respectively, which can tailor the oxidative dehydrogenation activity of the nanocarbons.

"As an efficient, metal-free catalyst, we have unraveled the roles of nitrogen dopants in both dehydrogenation and hydrogenation for the first time," said Xie. "We believe that our findings provide valuable insights into the physical-chemical reaction mechanisms of nitrogen-doped carbon catalytic systems and offer theoretical guidance for the synthesis of highly effective carbon catalysts."

More information: Xuefei Zhang et al, Identification of role of nitrogen dopants in nanocarbon catalysis, *Carbon Future* (2024). [DOI: 10.26599/CF.2024.9200008](https://doi.org/10.26599/CF.2024.9200008)

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