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Single atom catalyst

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AmirMahdi Tavassoli was born in 1994 and holds a Diploma in Mathematics with excellent grades and a bachelor's degree in applied chemistry from the university of Malayer. During his Bachelor's, he worked on decolorizing organic compounds. AmirMahdi completed his master's degree in organic chemistry from the university of Bu-Ali Sina under the supervision of Professor Mohammad Ali Zolfigol, where he worked on magnetic nanoparticles and ionic liquids to synthesize organic compounds in the laboratory of organic chemistry. During this time, he participated in more than five national organic chemistry seminars. He continues his scientific research and works on multicomponent reactions and covalent organic frameworks.

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This feature focuses on a reagent chosen by a postgraduate, highlighting the uses and preparation of the reagent in current research.

Introduction

Single-atom catalyst (SAC) has become an emerging area of research in the field of catalysis in recent years [1]. SACs are considered an attractive alternative to conventional heterogeneous catalysts due to their high activity, selectivity, and stability [2, 3]. The concept of SACs is based on the synthesis of metal ions or small clusters immobilized on solid supports, which enhances the catalytic activity of the metal.

The history of the single metal atom that is supported on a solid material and acts as a heterogeneous catalyst, has been formally proposed in 2011 by Zhang et al [4]. They confirmed the high efficiency of platinum atoms supported on iron oxide for CO oxidation. However, there were earlier studies that suggested the presence of single metal atoms in other catalytic systems, such as ionic gold or platinum species on ceria for water-gas shift reaction [5] or oxidized cobalt and iron species on functionalized carbons for oxygen reduction reaction [6]. The term SAC has been coined later to describe the isolated metal atoms supported on a solid material.

SACs have numerous applications in catalysis, including in energy production [7], environmental remediation [8], and chemical synthesis [9]. One of the most popular applications is in the electrochemical oxygen reduction reaction (ORR) in fuel cells [10]. The ORR involves the reduction of oxygen molecules to water, which generates energy. SACs have shown significant promise in this application due to their high catalytic activity and selectivity, leading to improved fuel cell performance [11].

Additionally, SACs play a crucial role in environmental remediation by converting harmful pollutants such as nitrogen oxides (NO_x) and carbon monoxide (CO) into harmless compounds. For example, SACs can catalyze the reduction of NO_x to nitrogen gas, which is a vital step in controlling air pollution [12, 13].

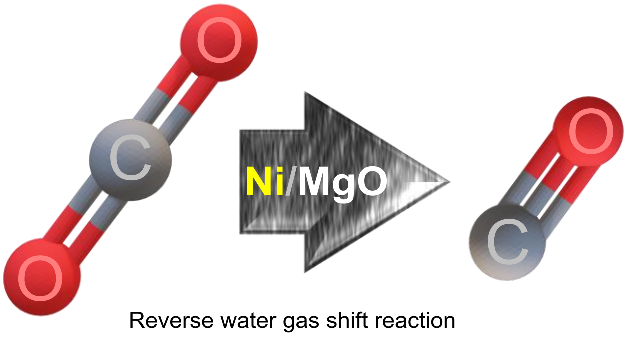
SACs also have applications in chemical synthesis, including the production of chemicals such as ethylene oxide, a critical raw material for the production of plastics [14]. SACs have shown improved selectivity and productivity in this application, leading to more efficient and sustainable chemical synthesis processes.

Literature surveys show that SACs are a promising area of research in catalysis due to their excellent properties. SACs have the potential to revolutionize the field of catalysis and contribute to a more sustainable future. They can also reduce the consumption of precious metals and minimize waste generation. SACs are a promising research direction that can bridge the gap between homogeneous and heterogeneous catalysis (**Scheme 1**) [15].

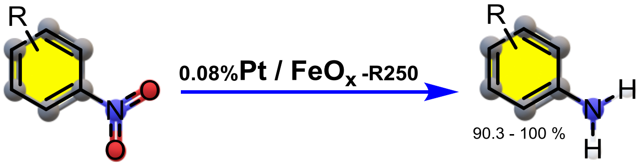
Scheme 1: SACs applications

Abstracts

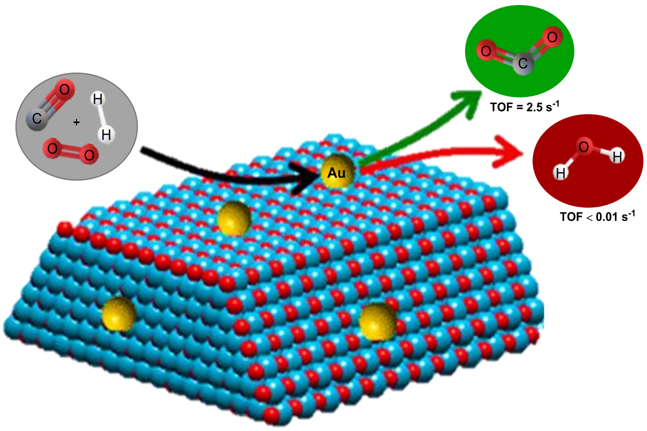
(A) Marie-Mathilde Millet and coworkers in 2019 reported the synthesis and characterization of a SAC that consists of isolated single Ni atoms substituted into a MgO structure. The single-atom catalyst shows high activity and stability for CO_2 activation through reverse water-gas shift (rWGS) reaction, which is an important reaction for CO_2 utilization and syngas production. The article also explains the catalytic mechanism of the SAC using density functional theory calculations, which reveal that the substitution of Mg atoms by Ni atoms on the surface of MgO reduces the CO_2 binding strength and promotes H_2 dissociation [16].



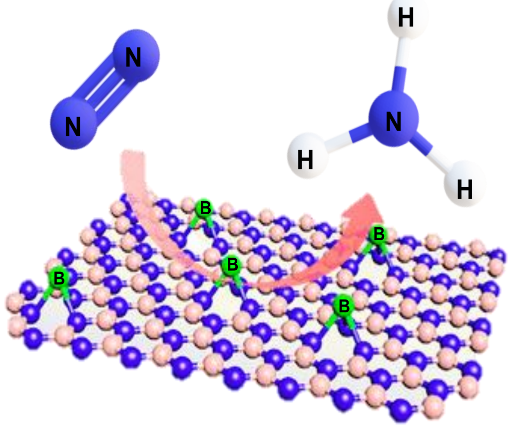
(B) In an article, published by Haisheng Wei and coworkers in 2014, the synthesis and characterization of a single-atom catalyst that consists of isolated single Pt atoms supported on FeO_x were done. The SAC shows high activity and chemo selectivity for the hydrogenation of various functionalized nitroarenes, which are important intermediates for agrochemicals, pharmaceuticals, and dyes. The article also explains the catalytic mechanism of the SAC using density functional theory calculations, which reveal that the positively charged Pt atoms with partially vacant 5d orbitals preferentially adsorb and activate nitro groups [17].



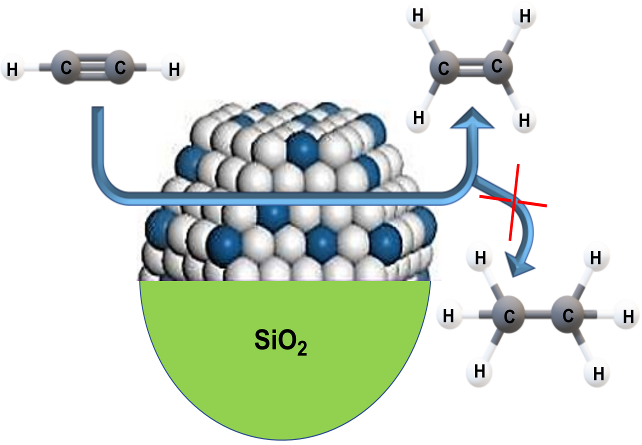
(C) In 2015, Botao Qiao and coworkers reported the synthesis and characterization of a single-atom catalyst that consists of isolated single Au atoms supported on CeO_2. The single-atom catalyst shows high activity, selectivity, and stability for preferential oxidation of CO (PROX) in the H_2-rich stream, which is an important reaction for producing clean H_2 for fuel cells. The mentioned article also explains the catalytic mechanism of the single-atom catalyst using density functional theory calculations, which reveal that the positively charged Au atoms with partially vacant 5d orbitals preferentially adsorb and activate CO molecules [18].



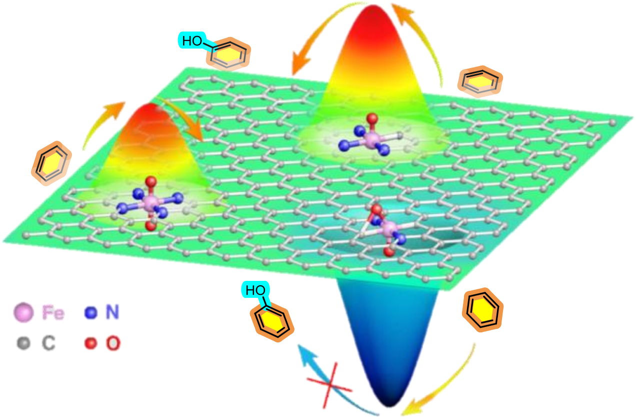
(D) Chongyi Ling and colleagues in 2018 reported a new metal-free catalyst that can convert nitrogen gas into ammonia using visible light. The catalyst is made of a single boron atom attached to a carbon-nitrogen sheet. The authors have used computer simulations for showing how the catalyst works and compare it with other existing catalysts. They claim that their catalyst is low-cost, stable, and eco-friendly. They have also suggested that their catalyst can use visible light as an energy source for nitrogen fixation, which is more abundant and sustainable than electricity or heat. They compare their catalyst with other metal-free or solar-driven catalysts that have been rarely explored for nitrogen fixation. [19].



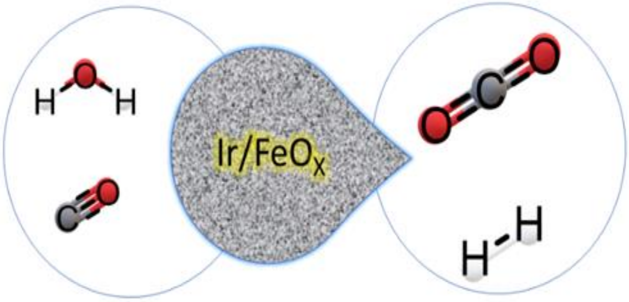
(E) Guang Xian Pei and coworkers in 2015 reported the synthesis and characterization of a single-atom catalyst that consists of isolated single Pd atoms alloyed with Ag and supported on SiO_2. The single-atom catalyst shows high activity and selectivity for the hydrogenation of acetylene to ethylene in excess ethylene, which is an industrially important process for purifying ethylene feedstock. The article has also explained the catalytic mechanism of the single-atom catalyst using *in-situ* FTIR, XPS, microcalorimetry, and XANES techniques, which reveal that the alloying of Pd with Ag leads to electron transfer from Ag to Pd and restructuring of AgPd nanoparticles during the reduction processes. These effects are resulting in a lower binding energy of CO on Pd atoms and a higher selectivity to ethylene [20].



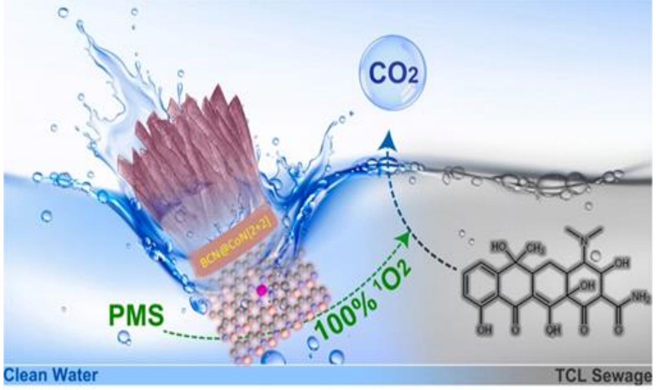
(F) In 2019 Yuan Pan and colleagues reported an article that explores how different coordination structures of Fe atoms with N and C atoms affect the catalytic performance of Fe-N_xC_y SACs for benzene oxidation, a reaction that can produce phenol as an important chemical intermediate. The authors have used a polymerization-regulated pyrolysis strategy to synthesize different Fe-N_xC_y catalysts with varying coordination numbers of Fe-N bonds. They find that four-coordinated Fe-N sites show the highest activity and selectivity for benzene oxidation while replacing N atoms with C atoms reduces the activity. They have explained the abovementioned facts by studying how oxygen interacts with Fe atoms and how it affects the reaction mechanism. The mentioned article reveals the importance of regulating the coordination structure of single-atom catalytic sites for optimizing their catalytic performance [21].



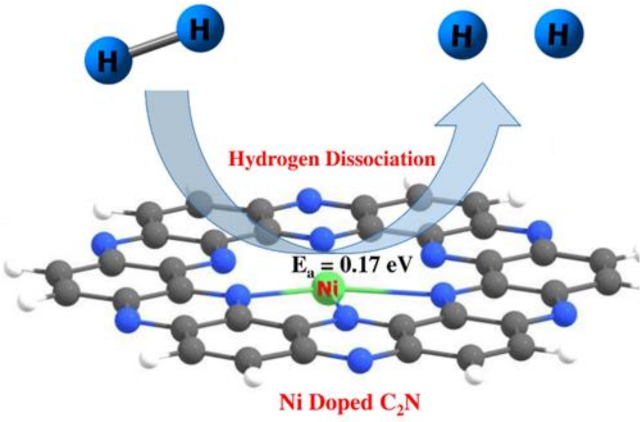
(G) Jian Lin and coworkers in 2013 reported the synthesis and characterization of a SAC that consists of isolated single Ir atoms supported on FeO_x. The SAC shows remarkable performance for the water gas shift (WGS) reaction, which is an important reaction for producing hydrogen from syngas. The article also explains the catalytic mechanism of the SAC using density functional theory calculations and *in-situ* characterization techniques, which reveal that the Ir atoms are positively charged and have partially vacant 5d orbitals that facilitate O_2 activation and CO adsorption [22].



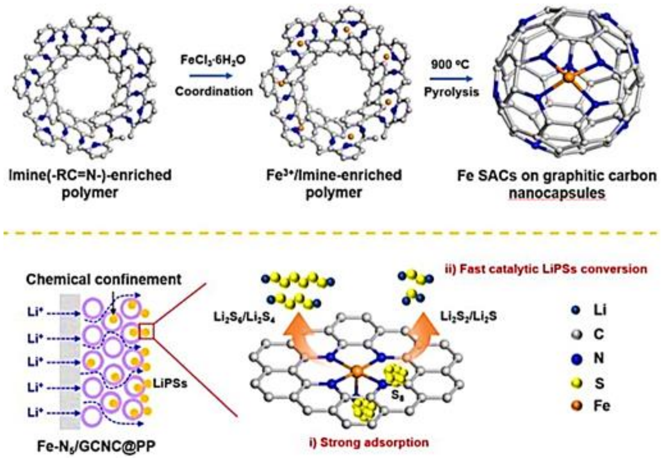
(H) Xue Zhao and colleagues reported a novel single-atom Co catalyst embedded in a BCN matrix for activating peroxymonosulfate (PMS) into singlet oxygen ($^1O_2$), a powerful oxidant for organic pollutant degradation. The authors have synthesized the Co-BCN catalyst by pyrolyzing a metal-organic framework precursor and characterized its structure and properties. They find that the single-atom Co sites can efficiently convert PMS into $^1O_2$ with a 100% conversion rate and high stability under various reaction conditions. They have also revealed the catalytic mechanism by using density functional theory calculations and radical trapping experiments. The article demonstrates that single-atom Co-BCN is a promising catalyst for environmental remediation applications [23].



(I) Ahmed Bilal Shah and coworkers presented a theoretical study of SACs of transition metals (Fe, Co, and Ni) doped on the C_2N surface for hydrogen dissociation reaction, a key step for hydrogen production and storage. The authors have used density functional theory calculations to evaluate the stability, electronic properties, and catalytic performance of different SACs on the C_2N surface. They find that Fe@C_2N is the most efficient catalyst among the three metals, with a low activation barrier of 0.36 eV and a high charge transfer between the metal atom and the C_2N surface. They also compare their results with previous studies on noble metal SACs and find that Fe@C_2N has a comparable or better catalytic activity than them. The article suggests that transition metal SACs on the C_2N surface are promising candidates for hydrogen dissociation reaction [24].



(J) Songjie He and colleagues reported a novel SAC of iron (Fe) coordinated by nitrogen (N) atoms and supported on graphitic carbon for enhancing the polysulfide conversion in lithium-sulfur batteries. The authors have synthesized the asymmetric N-coordinated Fe SAC by a facile pyrolysis method and characterized its structure and electrochemical properties. They have found that the asymmetric N-coordinated Fe SAC can effectively catalyze the redox reactions of polysulfides and suppress their shuttle effect, leading to improved battery performance. They have also investigated the catalytic mechanism by using density functional theory calculations and electrochemical impedance spectroscopy. The mentioned article demonstrates that asymmetric N-coordinated Fe SAC is a promising catalyst for lithium-sulfur batteries [25].



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