

Can acetylene be hydrogenated to ethylene?

Nature Catalysis 6, 1005-1015 (2023) Cite this article The hydrogenation of coal-based acetylene to ethylene is an important approach to establishing a non-oil route to ethylene production, yet it suffers from high H₂ consumption as well as a high energy input.

Why is selective hydrogenation of acetylene important?

This process circumvents the need for H₂ in the classical route and opens avenues for energy-efficient acetylene hydrogenation by water at low temperature. The selective hydrogenation of acetylene to ethylene involves high H₂ consumption as well as a high energy input.

Is hydrogenation of coal-based acetylene a viable non-oil route to ethylene production?

Provided by the Springer Nature SharedIt content-sharing initiative The hydrogenation of coal-based acetylene to ethylene is an important approach to establishing a non-oil route to ethylene production, yet it suffers from high H₂ consumption as well as a high energy input.

What is H₂ free acetylene hydrogenation?

Here we report a H₂-free acetylene hydrogenation process achieved by directly using water as the hydrogen source and low-cost CO as the oxygen acceptor over a Au/a-MoC catalyst. The process delivers over 99% acetylene conversion and a high ethylene selectivity of 83% at 80 °C, surpassing the hydrogenation process using H₂ as the hydrogen source.

What is acetylene semi-hydrogenation?

The selective hydrogenation of acetylene to ethylene involves high H₂ consumption as well as a high energy input. Now, a thermocatalytic process for acetylene semi-hydrogenation using H₂O as H source and CO on a Au/a-MoC catalyst is introduced.

Why is acetylene hydrogenation dangerous?

At the same time, excessive hydrogen as a hydrogen source can lead to unintended over-hydrogenation of ethylene and safety issues. In recent years, ionic liquid catalysts and metal-support interaction (MSI) have been widely used in acetylene hydrogenation.

The catalytic hydrogenation reaction has significant applications in the energy, chemistry, and pharmaceutical industries 1,2,3. For example, chemical products such as alkanes, alkenes, alcohols ...

Ethylene is an important feedstock for various industrial processes, particularly in the polymer industry. Unfortunately, during naphtha cracking to produce ethylene, there are instances of acetylene presence in the product stream, which poisons the Ziegler-Natta polymerization catalysts. Thus, appropriate process modification, optimization, and in ...

Selective hydrogenation plays an important role in the chemical industry and has a wide range of applications, including the production of fine chemicals and petrochemicals, pharmaceutical synthesis, healthcare product development, and the synthesis of agrochemicals. Pd-based catalysts have been widely applied for selective hydrogenation due to their unique ...

In this work, a particle-resolved computational fluid dynamics model of the acetylene hydrogenation process is developed to investigate the effects of catalyst particle structures on the reaction-diffusion behaviors aiming to improve selectivity toward target ethylene.

The semi-hydrogenation of acetylene ($C_2H_2 + H_2 = C_2H_4$, $\Delta H = -172 \text{ kJ mol}^{-1}$) is a well-studied reaction that is important for purification of ethylene, C_2H_4 , feed used in polyethylene production.

Well-defined atomically dispersed metal catalysts (or single-atom catalysts) have been widely studied to fundamentally understand their catalytic mechanisms, improve the catalytic efficiency, increase the abundance of active components, enhance the catalyst utilization, and develop cost-effective catalysts to effectively reduce the usage of noble metals. Such single ...

In this work, the H_2 dissociation and acetylene hydrogenation on Cu doped $CeO_2(111)$ were studied using density functional theory calculations. The results indicated that Cu doping promotes the formation of oxygen vacancy (Ov) which creates Cu/O and Ce/O frustrated Lewis pairs (FLPs). With the help of Cu/O FLP, H_2 dissociation can firstly proceed via a heterolytic ...

This comprehensive review explores recent electrochemical energy conversion and storage advancements, focusing on revolutionary catalyst strategies. The discussion ...

Semi-hydrogenation of acetylene in an ethylene-rich stream is an industrially important process. ... More Efficient Supercapacitor with High Performance for Energy storage and Device, Better Li ...

The selective hydrogenation of acetylene to ethylene in ethylene-rich gas streams is an important process in the manufacture of polyethylene. Conventional thermal hydrogenation routes require ...

In this work, the hydrogenation of acetylene on the $Pd_2/g-C_3N_4$ catalyst is investigated by the density functional theory (DFT) and quantum theory of atoms in molecules (QTAIM) calculations. The pre-reactant (R), transition states (TSs), and the intermediates (IMs), involved in the hydrogenation process, are characterized from the point of view of energy and ...

The energy system of industrial process, particularly in the petrochemical industry, consumes most of the utility cost. In this paper, a superstructure of a large-scale ...

The kinetics of the selective hydrogenation of acetylene in the presence of an excess of ethylene has been

studied over a 0.05 wt. % Pd/a-Al₂O₃ catalyst. The experimental reaction conditions were chosen to operate under intrinsic kinetic conditions, free from heat and mass transfer limitations. The data could be described adequately by a Langmuir-Hinshelwood rate-equation ...

Sheth PA, Neurock M, Smith CM (2003) A first-principles analysis of acetylene hydrogenation over Pd(111). *J Phys Chem B* 107(9):2009-2017. Article CAS Google Scholar Xie X, Song X, Dong W et al (2014) Adsorption mechanism of acetylene hydrogenation on the Pd (111) surface. *Chin J Chem* 32(7):631-636

The rational regulation of catalyst active sites at atomic scale is a key approach to unveil the relationship between structure and catalytic performance. Herein, we reported a strategy for the controllable deposition of Bi on Pd nanocubes (Pd NCs) in the priority order from corners to edges and then to facets (Pd NCs@Bi). The spherical aberration-corrected ...

The hydrogenation of acetylene to ethylene represents the most effective method for removing acetylene from the ethylene feedstock and various metal catalysts, including nanoparticles of Cu, Pd ...

Renewable energy-based electrocatalytic hydrogenation of acetylene to ethylene (E-HAE) under mild conditions is an attractive substitution to the conventional energy-intensive industrial process ...

The ratio of activation barriers to ethylene desorption/adsorption processes, which determines the acetylene hydrogenation selectivity, can vary depending on the structure of palladium nanoparticles and the electronic state of Pd. ... Interesting features of this energy scheme are that the binding energy of acetylene is lower (0.61 eV or 59 kJ ...

Renewable energy-based electrocatalytic hydrogenation of acetylene to ethylene (E-HAE) under mild conditions is an attractive substitution to the conventional energy-intensive

The presence of unpurified acetylene in petroleum-derived cracking gas significantly affects industrial polyethylene production. Even trace amounts of acetylene can poison polymerization catalysts, compromising both their activity and the quality of the resulting polymer [[1], [2], [3]]. Therefore, selective catalytic hydrogenation has been widely implemented ...

Hydrogen storage properties and reactivity for hydrogenation of acetylene in a series of CeNi_{5-x}Ga_x (x = 0, 0.5, 0.75, 1, 1.25, 1.5) alloys and Mg₂Ni were determined and compared. The ...

The hydrogen storage properties of ErNi_{5-x}Al_x (x = 0, 0.5, 0.75, 1, 1.25, and 1.5) alloys were investigated by pressure-composition isotherms and in situ X-ray diffraction ...

Acetylene semi-hydrogenation is an effective strategy to remove trace acetylene impurities (0.5-2.0%) from the ethylene stream to avoid poisoning the Ziegler-Natta catalyst. ...

Hydrogen storage properties and reactivity for hydrogenation of acetylene in a series of CeNi_{5-x}Ga_x and Mg₂Ni alloys were determined and compared and showed that the absorbed hydrogen in CeNi_{3.75}Ga_{1.25} improved reactivity. ABSTRACT Hydrogen storage properties and reactivity for hydrogenation of acetylene in a series of CeNi_{5-x}Ga_x ($x = 0, 0.5, \dots$

Acetylene (systematic name: ethyne) is the chemical compound with the formula C₂H₂ and structure H-C≡C-H is a hydrocarbon and the simplest alkyne. [8] This colorless gas is widely used as a fuel and a chemical building block. It is unstable in its pure form and thus is usually handled as a solution. [9] Pure acetylene is odorless, but commercial grades usually have a ...

d, Optimized potential energy surfaces of acetylene hydrogenation reaction over Ni₁Cu₂/g-C₃N₄ with energy reference of acetylene and hydrogen molecule in the gas phase. The dashed line ...

Semihydrogenation of trace acetylene in an ethylene gas stream is a vital step for the industrial production of polyethylene, in which Pd single-site catalysts (SSCs) have great potential. Herein, two Pd SSCs with ...

The hydrogen storage properties of ErNi_{5-x}Al_x ($x = 0, 0.5, 0.75, 1, 1.25, \text{ and } 1.5$) alloys were investigated by pressure-composition isotherms and in situ X-ray diffraction measurements under a hydrogen atmosphere. Catalytic reactivities toward the hydrogenation of alkynes (acetylene and propyne) over ErNi_{5-x}Al_x ($x = 0, 1, \text{ and } 1.5$) alloys were also studied and the contribution of ...

The hydrogen storage properties of ErNi_{5-x}Al_x ($x = 0, 0.5, 0.75, 1, 1.25, \text{ and } 1.5$) alloys were investigated by pressure-composition isotherms and in situ X-ray diffraction measurements under a hydrogen atmosphere. Catalytic reactivities toward the hydrogenation of alkynes (acetylene and propyne) over ErNi_{5-x}Al_x ($x = 0, 1, \text{ and } 1.5$) alloys were also studied ...

Acetylene semi-hydrogenation is a vital process where the utilization of supported isolated Pd atoms as catalytic active sites is promising due to their unique reactivity and metal atom efficacy. In particular, doping Pd single atoms at different sites on metal-oxide surfaces provides an opportunity to regulate their local coordination environments and modulate their electronic and ...

The energy profile of acetylene hydrogenation to ethane over this Pd cluster is shown in Fig. 4b, and the corresponding optimized configurations of surface intermediates and transition states are ...

To obtain a catalyst based on a non-precious metal that can replace traditional palladium-based selective catalysts of acetylene hydrogenation, the catalytic performances of two different configurations of a B₁₂N₁₂ cluster doped with a single nickel atom were studied by a density functional theory computational approach. After analysing the effect that the adsorption ...

This comprehensive review explores recent electrochemical energy conversion and storage advancements, focusing on revolutionary catalyst strategies. ... Hong X, Wei S, Wu Y, Li Y (2017) Single Ni sites distributed

on N-doped carbon for selective hydrogenation of acetylene. Chem Commun 53:11568-11571. Article Google Scholar

Ambient-condition acetylene hydrogenation to ethylene (AC-AHE) integrated with acetylene production from coal and natural gas, is a promising non-oil route for ethylene production with a low ...

These materials were then tested as catalysts for acetylene hydrogenation to ethylene. Science, this issue p. 560. View. Show abstract. ... For stationary energy storage systems, the feasibility ...

The main problem in the use of monometallic palladium catalysts is a high ethane yield. Researchers consider two possible routes of ethane formation: the direct hydrogenation ...

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