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COMMUNICATION
Zhenhai Wen *et al.*
An electrochemically neutralized energy-assisted low-cost acid-alkaline electrolyzer for energy-saving electrolysis hydrogen generation

An advanced three-dimensionally ordered macroporous $NiCo_2O_4$ spinel as a bifunctional electrocatalyst for rechargeable Zn–air batteries†

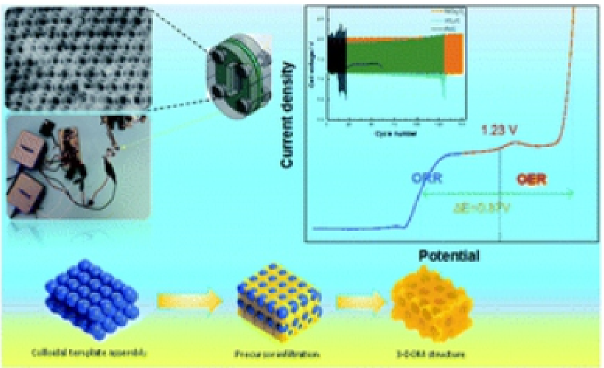
Check for updates

José Béjar,[a] Lorena Álvarez-Contreras,[b] Janet Ledesma-García,[c] Noé Arjona *[a] and Luis Gerardo Arriaga*[a]

⊕ Author affiliations

Abstract

In this work, highly active $NiCo_2O_4$ spinels with three-dimensionally ordered macroporous (3DOM) structures were obtained using poly(methyl methacrylate) (PMMA) spheres as a template, in which the high surface area of the 3DOM spinel, the presence of multiple valences of Co and Ni species and the high Ni content improve the activity for the oxygen reactions, presenting a current density value similar to that obtained for benchmark Pt/C. Also, the spinel needs only 10 mV more overpotential compared with benchmark IrO_2/C to achieve 10 mA cm^{-2} during the oxygen evolution reaction (OER). The 3DOM spinel shows superior stability for both reactions, retaining 80.5 (for the ORR) and 100% (for the OER) of the initial current after 10 h, respectively. This 3DOM spinel is used as an air electrode in a rechargeable Zn–air battery, enabling an open-circuit potential of 1.44 V, which is similar to that obtained for Pt/C (1.46 V), while also displaying a similar performance (109 *vs.* 101 mW cm^{-2}). Moreover, because of its excellent activity as a bifunctional electrocatalyst, the 3DOM spinel displays a superior charge–discharge capability after being operated for 21 h, while successfully supplying the energy requirements of a multi-sensor, which is operated for more than 2 h.



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Design and analysis of a dead volume control for a solar Stirling engine with induction generator

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ABSTRACT

In this work, a power generation system dish/Stirling with cavity receiver and an electrical induction generator was simulated. We propose a control system using a variable-dead-volume and analyze its influence on the mechanical performance. A system with a dead volume of 160 cm^3 was designed to control the power and speed of the engine considering annual insolation, mechanical properties of the heater and the limits of frequency and voltage for the systems interconnected to the electricity network. The designed system achieves net efficient solar conversion to electric of 23.38% at an irradiance of 975 W/m^2 and allows an annual increase of 18% of the useful electrical energy compared to a system without control.

1. Introduction

With increasing power demand, and growing concerns over energy security and environmental impact, deployment of renewables has been accelerating and is expected to be continued. This growth depends on subsides to facilitate deployment and drive further cost reductions [1]. In particular, the high temperature solar thermal technology is very promising and driven since it is an excellent candidate to produce electrical energy. It turns out that among all the solar thermal technologies the dish Stirling one is the most efficient for electricity production. Indeed, Revy et al. studied the technical feasibility to produce electrical energy by plants with parabolic trough, dish Stirling and central tower solar technologies and found that the cheapest technology to produce electricity in India is the dish Stirling one [2]. In a parabolic dish commercial plant with a 30 kW Stirling power converter, this technology achieved a solar-to-grid-quality-electricity efficiency of 32% [3]. However the main disadvantages of the Stirling engines are their high cost, the sealing problems and the complicated power modulation [4,5]. Efforts to increase the profitability of this technology are focused in its production in large volumes and its operation with hydrogen or helium at high pressures in order to achieve higher power and greater electrical energy produced annually per system.

A Stirling engine is a heat engine which converts thermal energy to mechanical work by cyclic compression and expansion of the working fluid, most commonly hydrogen, helium or air. It is composed of three systems of high sophistication, complexity and cost: (1) engine, (2) heating provision, and (3) pre-heater. An essential safety feature is the micro-processor feedback between heater temperature and fuel supply rate. An engine operating with H_2/He requires an additional system to reserve and replenish. This technology still presents technical challenges to improve the gas sealing and the motor control for the modulation of the power [4,7]. Prospects in terms of cost, reliability and packaging envelope are not yet improved [6].

The Stirling engine performance depends on its geometrical and physical characteristics and the working fluid. In general, working with hydrogen or helium results in better efficiencies. However, Meijer shows numerical results comparing the power density of Stirling engines working with air and hydrogen/helium indicating that at low velocities, around 250 rpm, the difference between

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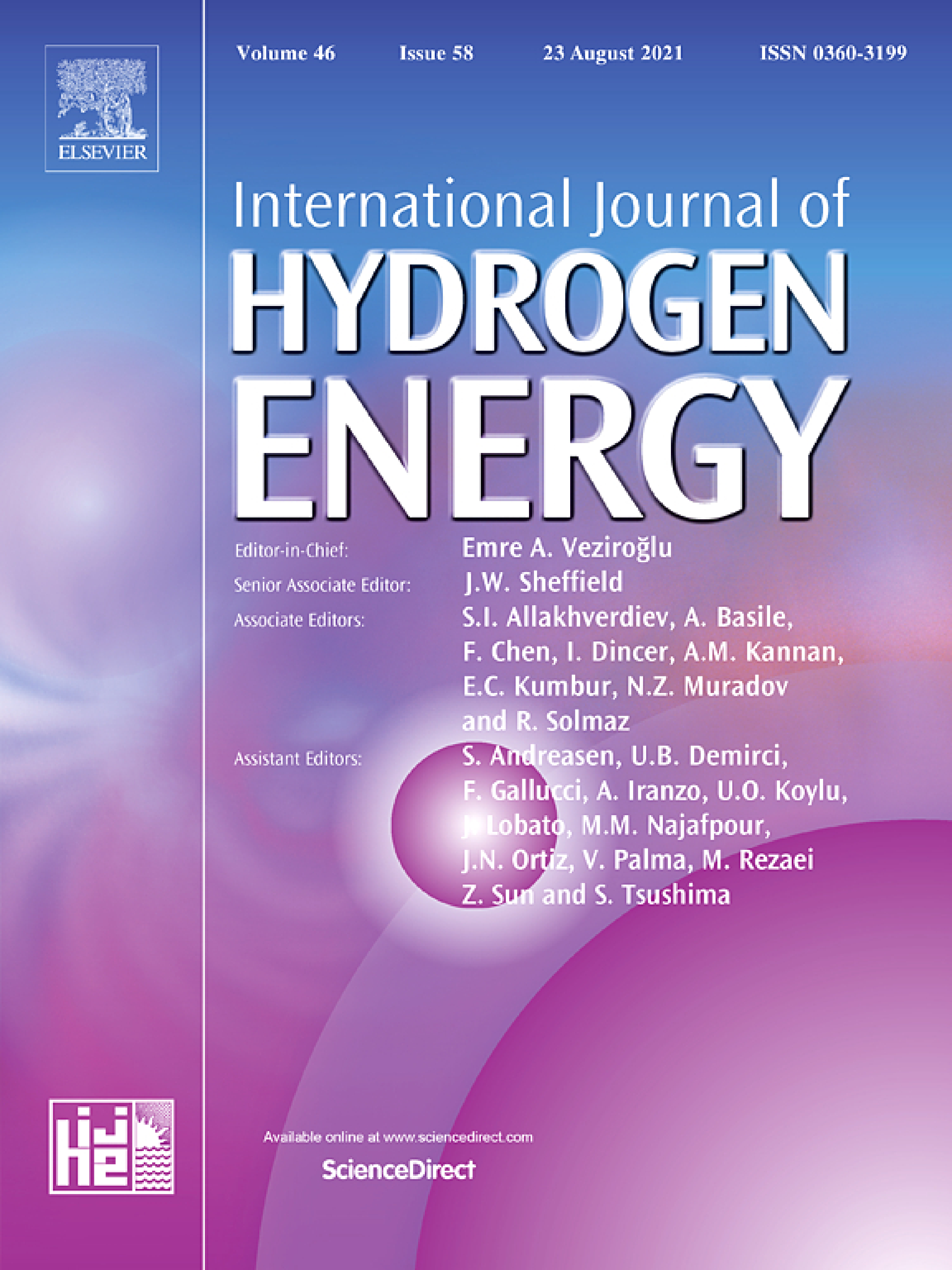

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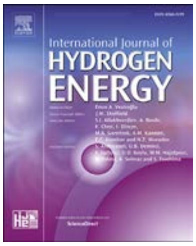

Optimization of the electrooxidation of aqueous ammonium sulfite for hydrogen production at near-neutral pH using response surface methodology

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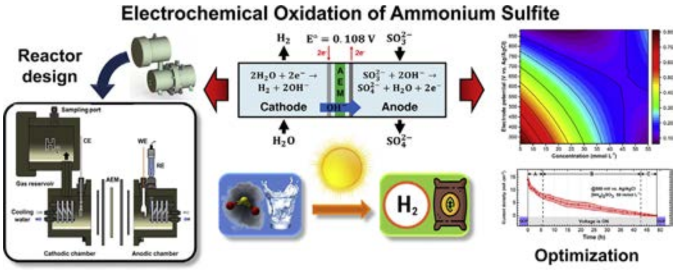
HIGHLIGHTS

- Batch electrooxidation of ammonium sulfite is optimized at slightly alkaline media.
- pH is stabilized in an electrochemical reactor by means of an anion exchange membrane.
- A second-order model for electrooxidation rate estimation is obtained.
- Long-term electrooxidation tests demonstrate robustness of the approach.

GRAPHICAL ABSTRACT



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Sulfite electrooxidation
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ABSTRACT

Sulfur-based thermochemical cycles, such as the hybrid sulfur-ammonia (HySA) cycle, offer a valuable approach in which hydrogen is produced by exploiting sulfur dioxide (potentially pollutant emissions) through the electrochemical oxidation of aqueous sulfite. In this study, the effect of pH on electrooxidation rate was assessed by comparing different reaction scenarios. Then, a Central Composite Design (CCD) combined with a Response Surface Methodology (RSM) was used to optimize batch electrooxidation of ammonium sulfite at near-neutral pH. Results show that the use of an anion exchange membrane (AEM) greatly improves sulfite electrooxidation rate while pH is effectively stabilized. Furthermore, a second-order model that relates applied potential and sulfite concentration with the normalized half-life of the reaction was obtained and verified experimentally at

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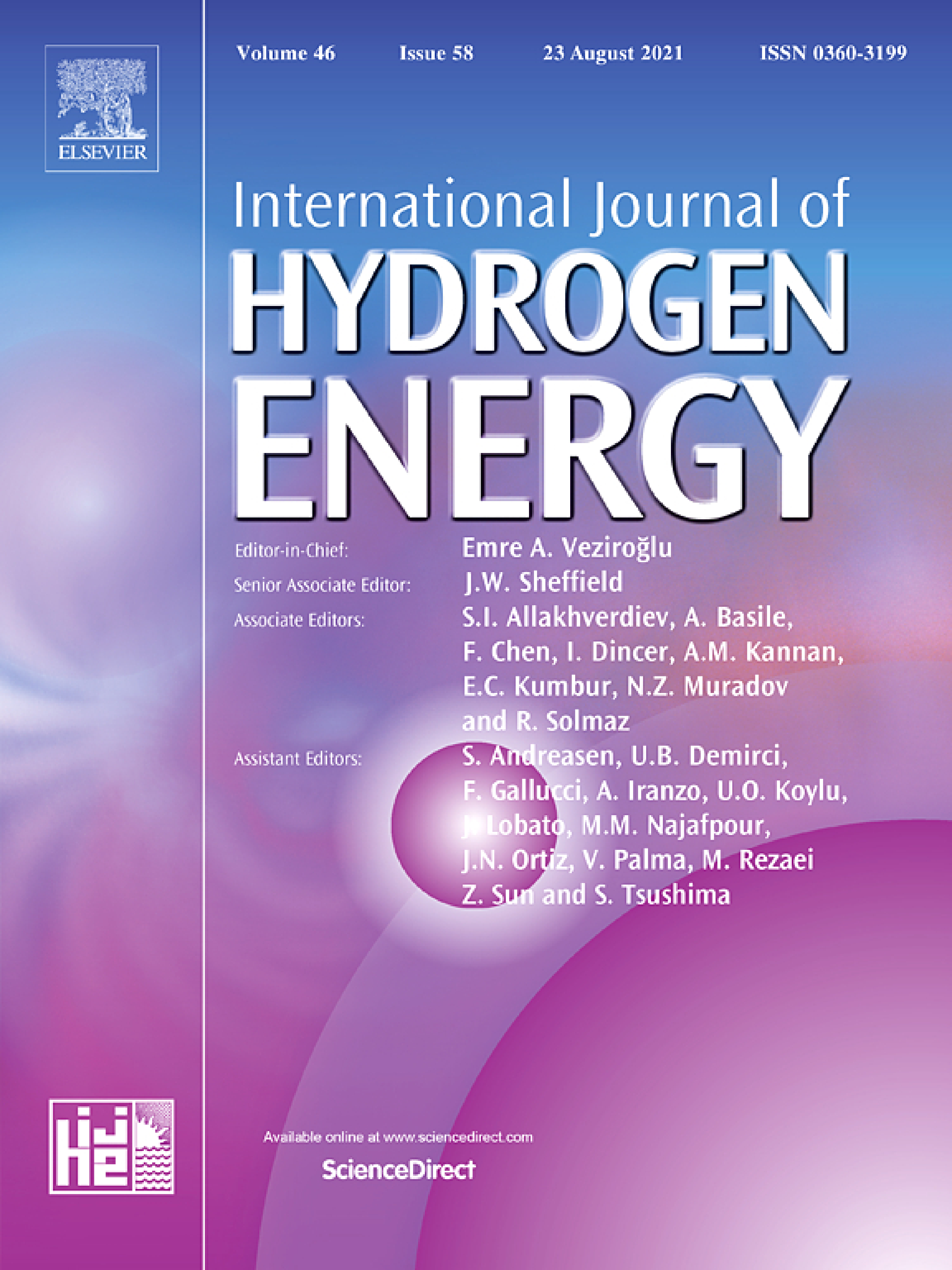

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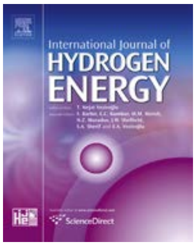

Na_2ZrO_3 stability under reforming/regeneration cycles during the steam reforming of ethanol with CO_2 absorption

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Absorption enhanced ethanol reforming
Na_2ZrO_3
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ABSTRACT

In this work Na_2ZrO_3 and a Ni–Al_2O_3 catalyst were used to evaluate the hydrogen production by the steam reforming of ethanol in combination with CO_2 absorption (SREA). The Na_2ZrO_3 was synthesized by the solid state method with a $Na_2CO_3/ZrO_2 = 1:1$ molar ratio and calcined at 900 °C in air. A 25% W Ni–Al_2O_3 catalyst was synthesized by incipient impregnation and calcined at 900 °C in air. During reforming, operating conditions were: $H_2O/C_2H_5OH/Na_2ZrO_3 = 6:1:2.5$ feed molar ratio, $T = 600$ °C, $SV = 414\ h^{-1}$. Na_2ZrO_3 absorbent was separately regenerated at 900 °C and air. Experimental reaction results indicate a high stability of Na_2ZrO_3 under 10 consecutive reforming/regeneration cycles allowing to reach SREA equilibrium values. H_2 production reached 91.3% mol of accompanied by 5.2 CO_2, 1.2 CO, and 2.2 CH_4% mol for each of the 10 consecutive cycles. These results show Na_2ZrO_3 high stability towards multi-cycle SREA operation.

Introduction

Today fossil fuels dominate the power generation worldwide, especially in the transport sector. However, this has significantly contributed to an increase of CO_2 emissions to the atmosphere with an important impact on climate change [1]. The continuous release of CO_2 can be alleviated by changing to renewable energy sources or preventing the release of CO_2 into the atmosphere during the combustion of hydrocarbons. This can be achieved through technology that generates energy without the use of fossil fuels or by converting renewable compounds such as methanol, ethanol or biodiesel directly into hydrogen for its use in fuel cells [2,3]. Currently, the main process to produce large scale H_2 is by catalytic steam methane reforming (SMR), which involves a step for the separation of CO_2 such as: pressure swing adsorption or amines [4]. However, in order to make a significant improvement in this process, research has been conducted related to the separation of CO_2 at high temperatures in order to increase its efficiency. To achieve this, a series of solid CO_2 absorbents with specific properties have been developed, which

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Chapter 5

Chemical Reactivity Properties and Bioactivity Scores of the Angiotensin II Vasoconstrictor Octapeptide

Norma Flores-Holguín, Juan Frau and Daniel Glossman-Mitnik

Abstract

Eight density functionals, CAM-B3LYP, LC-ωPBE, M11, MN12SX, N12SX, ωB97, ωB97X, and ωB97XD, in connection with the Def2TZVP basis set were assessed together with the SMD solvation model for the calculation of the molecular and chemical reactivity properties of the angiotensin II vasoconstrictor octapeptide in the presence of water. All the chemical reactivity descriptors for the systems were calculated via conceptual density functional theory (CDFT). The potential bioavailability and druggability as well as the bioactivity scores for angiotensin II were predicted through different methodologies already reported in the literature which have been previously validated during the study of different peptidic systems.

Keywords: angiotensin II, conceptual DFT, chemical reactivity, drug-likeness features, bioactivity scores

1. Introduction

In order to consider peptides and related compounds as the starting point for the development of medical drugs, it is mandatory to acquire a knowledge about their chemical reactivity properties as well as the bioactivity associated with them. From the basics of medicinal chemistry, it is known that drugs exert their effect by interacting with the active site of a receptor which is generally a protein [1]. These interactions rely on the different kinds of bindings between the pharmacophore and the chemical groups present in the active site and thus intimately related to their chemical reactivity from a molecular perspective [2, 3]. One of the most powerful tools to understand the chemical reactivity of interacting molecular systems within computational chemistry is probably the conceptual density functional theory (CDFT) [4, 5], also called chemical reactivity theory, which allows to accomplish this task by resorting to several global and local descriptors which are in turn related to variations in the electronic densities of the studied systems.

On the basis of the previous considerations, the objective of this work is to study the chemical reactivity of an octapeptide known as angiotensin II that acts