

Quadricyclane solar energy storage





Overview

Is electronic relaxation of quadricyclane after exciting in the ultraviolet (201 nanometres)?

Here we study the electronic relaxation of quadricyclane after exciting in the ultraviolet (201 nanometres) using time-resolved gas-phase extreme ultraviolet photoelectron spectroscopy combined with non-adiabatic molecular dynamics simulations.

How do electronic excited quadricyclane molecules relax to the electronic ground state?

We identify two competing pathways by which electronically excited quadricyclane molecules relax to the electronic ground state. The fast pathway (<100 femtoseconds) is distinguished by effective coupling to valence electronic states, while the slow pathway involves initial motions across Rydberg states and takes several hundred femtoseconds.

What is the branching ratio of norbornadiene/quadricyclane products?

Both pathways facilitate interconversion between the two isomers, albeit on different timescales, and we predict that the branching ratio of norbornadiene/quadricyclane products immediately after returning to the electronic ground state is approximately 3:2.



Quadricyclane solar energy storage



A hydrocarbon molecule as supplier and energy storage solution ...

energy storage solution for solar energy April 19 2024, by Blandina Mangelkramer Calculated absorption strained quadricyclane. 2/4 "The conversion process is already known, however, research

Solar Energy Storage by Molecular Norbornadiene-Quadricyclane ...

Devices that can capture and convert sunlight into stored chemical energy are attractive candidates for future energy technologies. A general challenge is to combine efficient solar energy capture with high energy densities and energy storage time into a processable composite for device application. ...



Environmental Effects on the Norbornadiene-quadricyclane ...

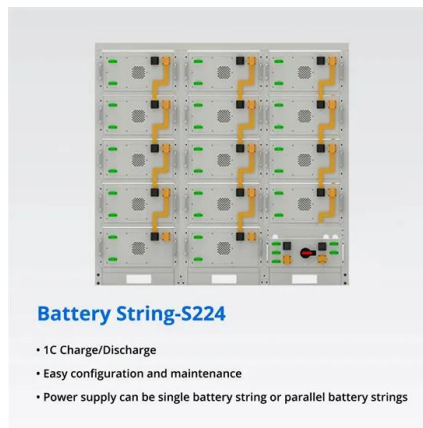
In the shift towards renewable energy sources, harnessing solar energy emerges as a pivotal focus due to the sun's abundance as an untapped energy reservoir [1,2]. Molecular photoswitches offer a promising, cost-effective avenue for potentially storing solar

Maximizing the Solar Energy Storage of the Norbornadiene-Quadricyclane

Abstract An attempt was made to maximize the solar energy storage in a norbornadiene (1)/quadricyclane (2) system, through the angling of mono-heteroatoms at C 1, C 2, or C 7



atoms of 1 and 2 and calculating the corresponding energies at the B3LYP/6-311++G(3df,2p) level of theory.



Solar Energy Storage: Competition between Delocalized Charge ...

Solar Energy Storage: Competition between Delocalized Charge Transfer and Localized Excited States in the Norbornadiene to Quadricyclane Photoisomerization
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Maximizing the Solar Energy Storage of the Norbornadiene-Quadricyclane

An attempt was made to maximize the solar energy storage in a norbornadiene (1)/quadricyclane (2) system, through the angling of mono-heteroatoms at C1, C2, or C7 atoms of 1



Unraveling Factors Leading to Efficient Norbornadiene-Quadricyclane

Factors Leading to Efficient Norbornadiene-Quadricyclane Molecular Solar-Thermal Energy Storage Systems , Developing half-life of the quadricyclane, and energy-storage density) by the



Engineering of Norbornadiene/Quadricyclane

The most impactful recent findings on how to engineer key properties of the NBD/QC system (photochemistry, energy storage, heat release, stability, and synthesis) are described as well as examples of test devices for solar energy capture and heat release. Conspectus Renewable energy resources are mostly intermittent and not evenly distributed ...

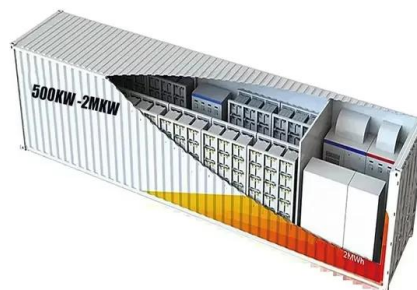


Norbornadiene-based photoswitches with exceptional ...

Norbornadiene-quadricyclane (NBD-QC) photoswitches are candidates for applications in solar thermal energy storage. Functionally they rely on an intramolecular [2+2] ...

Norbornadiene-quadricyclane -- an effective molecular system ...

The results of studies on intramolecular interconversions in systems of norbornadiene quadricyclane and their derivatives are classified and discussed. The mechanisms of the forward photoreaction and reverse thermal process in relation to the nature of the substituents and carbocycles, type of sensitizer and catalyst, and properties of the medium are ...



Norbornadiene/Quadricyclane (NBD / QC) and Conversion of Solar Energy

The molecular solar thermal-energy-storage system (MOST) application and its design of heat-release devices based on the NBD/QC system have been strongly evolving in the last years. However, also several new applications start to develop, making this photoswitch a versatile compound.



Liquid Norbornadiene Photoswitches for Solar Energy Storage

Due to high global energy demands, there is a great need for development of technologies for exploiting and storing solar energy. Closed cycle systems for storage of solar energy have been suggested, based on absorption of photons in photoresponsive molecules, followed by on-demand release of thermal energy. These materials are called solar thermal ...



Solar Energy Storage by Molecular Norbornadiene-Quadracycline

solar energy storage efficiencies of up to 3.8% combined with attractive energy storage densities of up to 0.48 MJ kg⁻¹. The combination of donor and acceptor units leads to an improved solar spectrum match with an onset of absorption of up to 529 nm and at 1/

Engineering of Norbornadiene/Quadracycline ...

This Account describes the most impactful recent findings on how to engineer key properties of the NBD/QC system (photochemistry, energy storage, heat release, stability, and synthesis) as well as examples of test ...



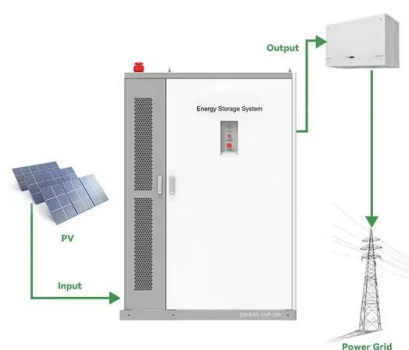


Solar energy storage at an atomically defined organic-oxide ...

Our atomically-defined solar-energy-storing model interface enables detailed studies of energy conversion processes at organic quadricyclane (CQC) storing 0.363 MJ/kg in form of chemical

Prospects of Improving Molecular Solar Energy Storage of the

We have investigated novel bicyclic diene molecular solar thermal energy storage systems that presently are the ones with the highest predicted energy density. Using a variety of different ab initio quantum chemical methods, we report storage energies, absorption spectra, and reaction barriers for the release of stored energy for a series of bicyclic dienes. ...



(PDF) Engineering of Norbornadiene/Quadricyclane ...

or solar thermal fuels (STF). Such molecules offer a promising solution for solar energy storage applications. norbornadiene - quadricyclane molecular solar-thermal energy storage systems. J

Ultrafast electronic relaxation pathways of the molecular

Alex, W. et al. Solar energy storage: competition between delocalized charge transfer and localized excited states in the norbornadiene to quadricyclane photoisomerization. J. Am.





Norbornadiene-Quadricyclane Photoswitches with Enhanced Solar

Norbornadiene absorbs in the UV region making it unsuitable for molecular solar thermal energy storage. A new series of visible light-absorbing norbornadienes were synthesized and evaluated. The stra

The Norbornadiene/Quadricyclane Pair as Molecular Solar Thermal Energy

1 Introduction 1.1 Molecular Solar Thermal (MOST) Systems The primary energy demand is expected to increase by about 1 % per year up to 2030 reaching 485 EJ for the world consumption in the Stated Policies Scenario. 1 However, the need to reduce climate-damaging emissions 2 urges the transition from fossil to renewable energy sources. 3 To master these ...



Norbornadiene-based photoswitches with exceptional combination of solar

Norbornadiene-quadricyclane (NBD-QC) photoswitches are candidates for applications in solar thermal energy storage. Functionally they rely on an intramolecular [2+2] cycloaddition reaction, which couples the S0 landscape on the NBD side to the S1 landscape on the QC side of the reaction and vice-versa. This commonly results in an unfavourable ...

Solar Energy Storage: Competition between Delocalized Charge ...

We describe for the first time the full reaction coordinate regarding the photoisomerization of red-absorbing norbornadienes (NBDs) to quadricyclanes (QCs). Our ...



Molecular Solar-Thermal Energy Storage: Molecular Design and ...

Behr A, Keim W, Thelen G, Scharf HD, Ressler I (1982) Solar energy storage with quadricyclane systems. J Chem Technol Biotechnol 32(6):627-630 Article Google Scholar Gassman PG, Patton DS (1968) Acid-catalyzed rearrangement of Product dependency



Norbornadiene-quadricyclane as an abiotic system for the storage ...

Data on the valence isomerisation of norbornadiene and its derivatives into the corresponding quadricyclanes published between 1990 and 2001 are considered and described systematically. The applicability of this reaction for the storage of solar energy is discussed. The bibliography includes 112 references.



Norbornadiene-quadricyclane system in the photochemical ...

Synthesis and Characterization of Carbon-Based Heterogeneous Catalysts for Energy Release of Molecular Solar Thermal Energy Storage Materials. ACS Applied Materials & Interfaces 2024, 16 (6)





Ultrafast electronic relaxation pathways of the molecular

The last example includes molecular solar thermal (MOST) energy storage solutions, whereby molecular isomers are exploited to absorb, store and later release solar ...



[Solar Energy Storage by Molecular ...](#)

A general challenge is to combine efficient solar energy capture with high energy densities and energy storage time into a processable composite for device application. Here, norbornadiene (NBD)-quadricyclane (QC) ...

Photochemical Energy Storage and Electrochemically Triggered Energy

A new photoelectrochemical infrared reflection absorption spectroscopy (PEC-IRRAS) experiment is presented, which allows monitoring of the complete energy storage and release cycle by in situ vibrational Spectroscopy. The two valence isomers norbornadiene (NBD) and quadricyclane (QC) enable solar energy storage in a single molecule system. We present ...



Norbornadiene-quadricyclane -- an effective molecular system ...

The results of studies on intramolecular interconversions in systems of norbornadiene quadricyclane and their derivatives are classified and discussed. The mechanisms of the forward photoreaction and reverse thermal process in relation to the nature of the substituents and carbocycles, type of sensitiser and catalyst, and properties of the medium are ...



Solar energy storage at an atomically defined organic-oxide ...

In this work, we report on the assembly of an operational solar-energy-storing organic-oxide hybrid interface, which consists of a tailor-made molecular photoswitch and an ...



Steric effect studies on solar energy storage of norbornadiene

The aim of this research is to determine the possible solar energy storage in the norbornadiene (1) / quadricyclane (2) system, through involving steric effects on various position of

Surface chemistry of 2,3-dibromosubstituted norbornadiene/quadricyclane

The adsorption behavior, energy release, and surface chemistry on Ni(111) is studied using high-resolution X-ray photoelectron spectroscopy (HR-XPS), UV photo Electron Spectroscopy, and density functional theory calculations. Dwindling fossil fuels force humanity to search for new energy production routes. Besides energy generation, its storage is a crucial ...



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