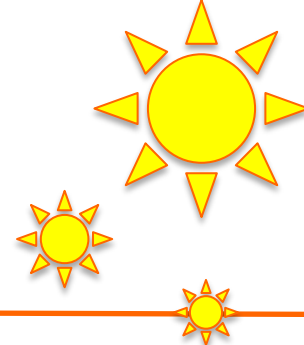




**Center for Exploitation of Solar Energy &
Department of Chemistry, University of Copenhagen**



- Mogens Brøndsted Nielsen (*Organic synthesis*)
- Kurt V. Mikkelsen (*Theory*)
- Henrik G. Kjærgaard (*Spectroscopy*)

Sustainable Energy for All
– A Brief Overview of Solar Energy
and some of our research activities in this field

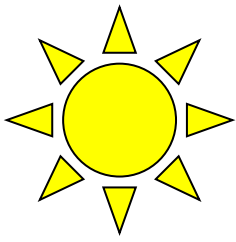


Annual global energy demand

... is expected to increase by a factor of 1.5 from 2007 to 2035

Challenges

- **Ready access to sustainable energy sources all over the world for cooking, heating, *etc.***
- **Economic growth equitable and addressing growing energy demand**
- **Reduction of global emissions**



Challenges

- Ready access to sustainable energy sources all over the world for cooking, heating, *etc.*
- Economic growth equitable and addressing growing energy demand

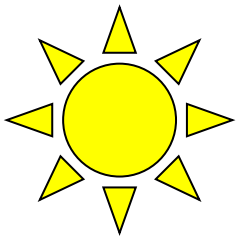
Sunlight

... is the the most abundant carbon-neutral energy source available on Earth.

The amount of energy from the sun hitting Earth in 1 hour is more than the total global consumption of energy in one year!

- Reduction of global emissions

Can we use **closed energy cycles** with no emissions of CO₂ or other pollutants?



Uses of Sunlight *capture – conversion – storage*

- **Photovoltaics:** *Direct conversion into electricity*
- **Concentrated solar power:** *Large beams of sunlight are focused into a small beam using mirrors or lenses. Heat transfer fluid systems, for example to drive steam turbines ... or for water heating*
- **Photocatalysis** – *for example conversion of water into hydrogen and oxygen or synthesis of other solar fuels. Combustion of H_2 produces only H_2O (carbon-neutral method of storing solar energy). Storage of H_2 gas is a major challenge (one method is as solid hydrides) and maybe better to store the solar energy directly as batteries (?)*

Solar powered hot water systems utilize solar energy to heat water.

In certain areas, 60 to 70% of water used domestically for temperatures as high as 60 °C can be made available by solar heating.

Solar Energy – Advantages

Many different purposes: It can be used to generate electricity in places that lack a grid connection, for distilling water in Africa, or to power satellites.

Building materials: With flexible thin-film solar cells, solar power may be integrated into the material of buildings

No over-consumption: Solar energy is sustainable - there is no way we can over-consume.

No pollution: Harnessing solar energy does generally not cause pollution. However, there are emissions associated with the manufacturing, transportation and installation.

Availability: Solar energy is available all over the world.

Low Maintenance: Most solar power systems do not require a lot of maintenance.

Silent: No noise associated with photovoltaics.

Solar Energy – Drawbacks

Space: The global mean power density for solar radiation is more than any other renewable energy source, but not comparable to oil, gas and nuclear power.

Pollution: Some manufacturing processes are associated with greenhouse gas emissions.

Exotic materials: Certain solar cells require materials that are expensive and rare in nature, either cadmium telluride (CdTe) or copper indium gallium selenide (CIGS).

Cost: Average cost per kWh is a factor of 2-3 higher than other sources

Intermittent energy source: Access to sunlight is limited at certain times. However, solar power has fewer problems than wind power in this regard.

→ **Storage:** mismatch of supply and demand

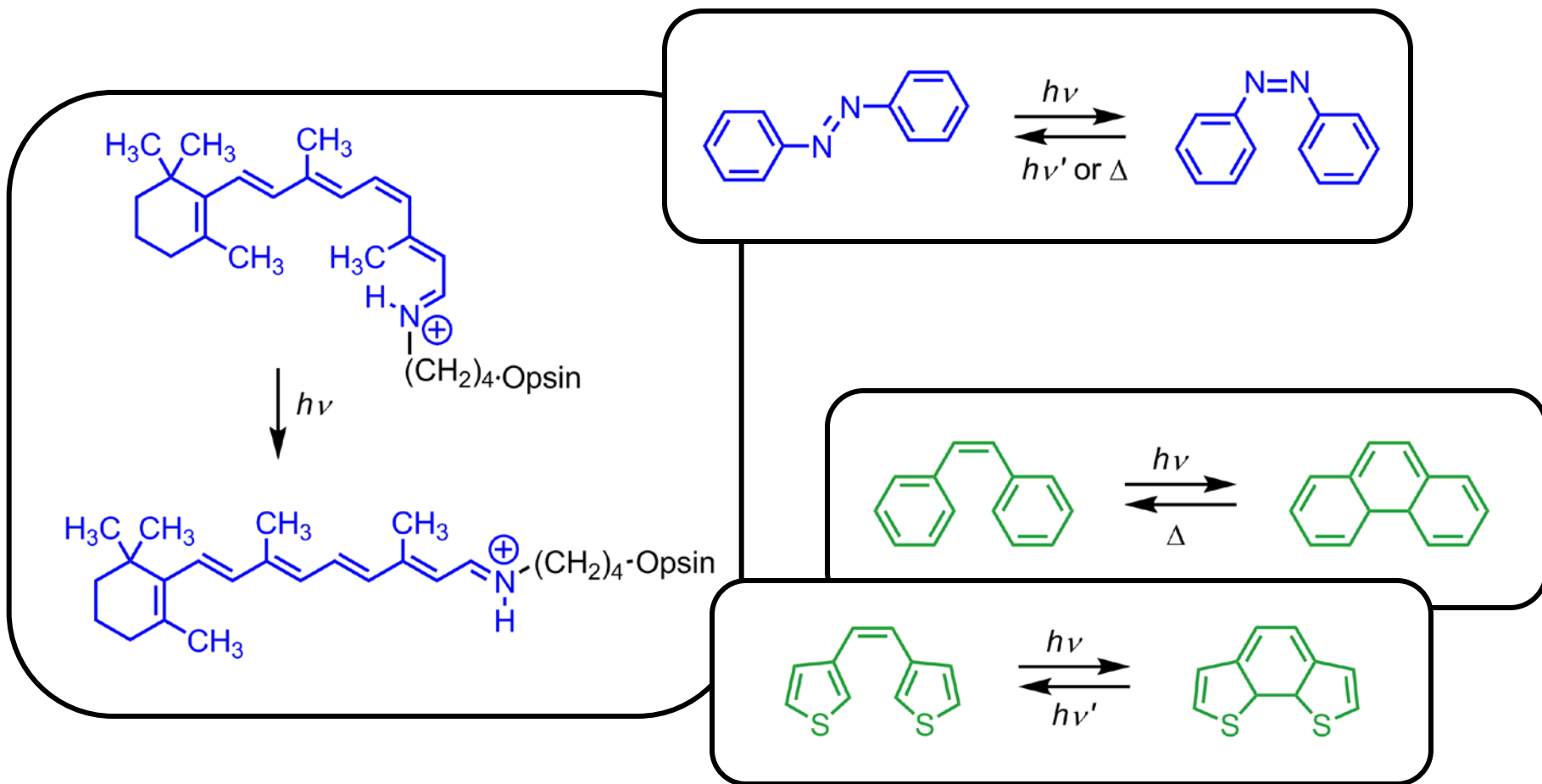
How is the energy stored?

When you speak of the sun, it shines.

Then I don't understand why we don't speak about it! - Storm P.

Robert Storm Petersen (1882-1946; Danish cartoonist, painter and humorist)

Molecular Photoswitches / Photochromic Molecules



Cis-trans isomerizations

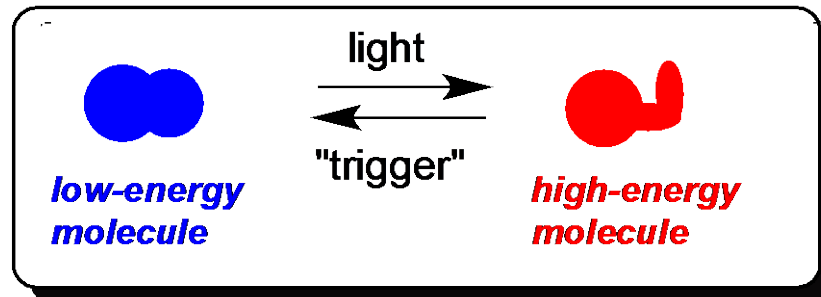
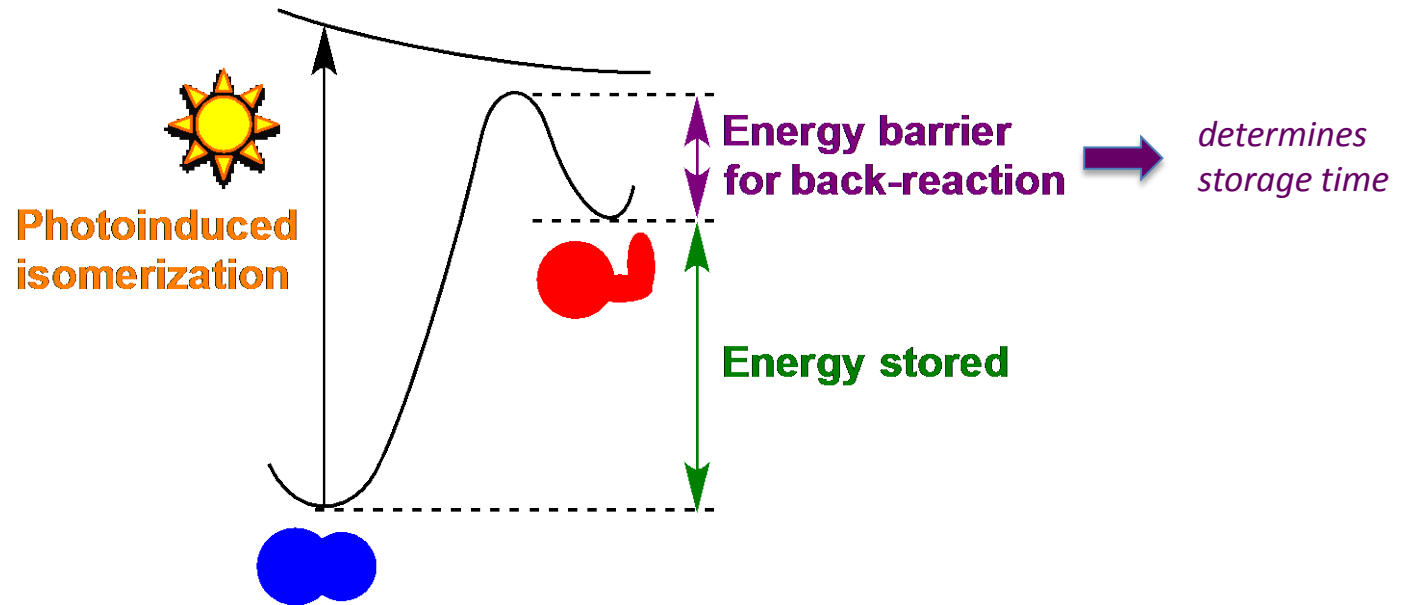
Electrocyclic reactions

... changes in molecular structure upon irradiation

Energy Storage using Photochromic Molecules

– Closed Energy Cycle with No CO₂ Emissions or Other Pollutants

Light absorption – Storage – Energy release on demand



Challenges

- How do we design photochromic molecules with sufficiently high energy densities?
- How is the energy-releasing back-reaction put on stand-by? ... *energy storage*
- How do we avoid photodegradation of molecules over many cycles?

...

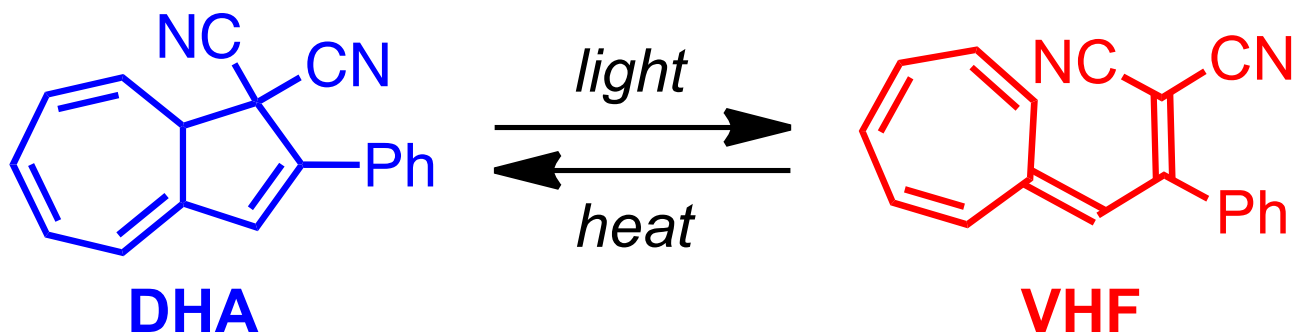
... Material with energy density of 1 MJ / kg

- Heat release of 1 MJ can be used to bring 3 L of water from room temperature to the boiling point
- Harvesting light during the day and releasing heat during the night:
 - maintaining 1 m³ at 19 °C with outside temperature of -6 °C requires ca. 3 kg of solar thermal battery (when using foam insulation)

T. R. Kucharski, Y. Tian, S. Akbulatov, R. Boulatov, *Energy Environ. Sci.* **2011**, 4, 4449-4472.

Compare: Li ion batterier < 1 MJ / kg

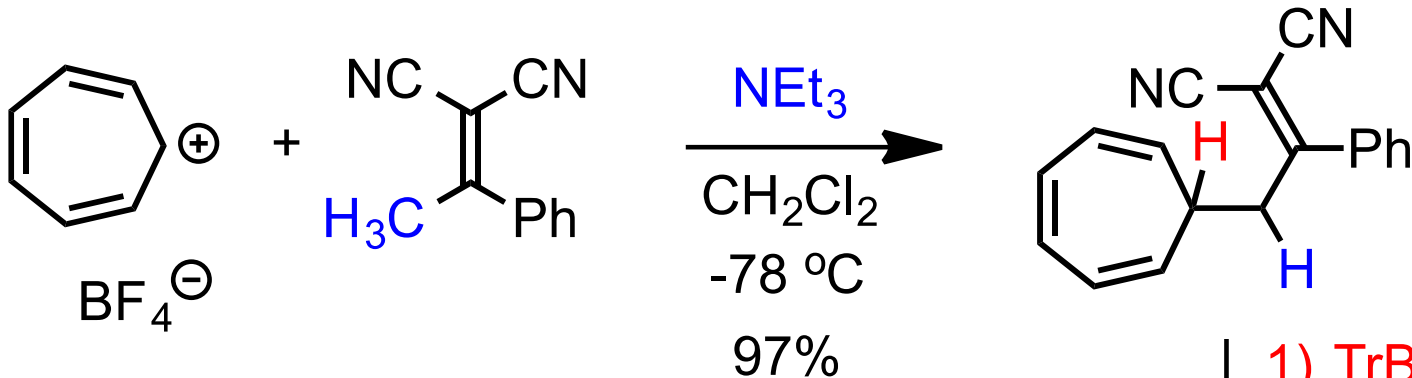
Another Candidate Molecule: Dihydroazulene (DHA)



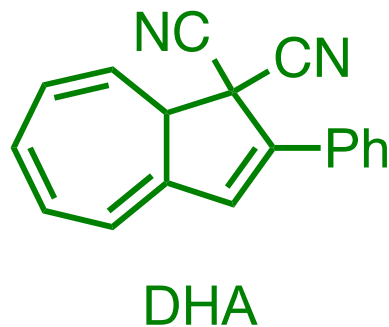
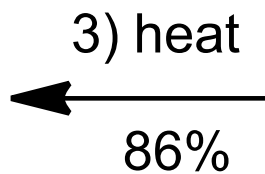
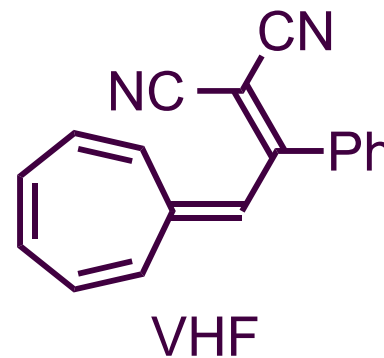
Energy storage: 0.11 MJ / kg

... We need to modify the molecule to increase this value!

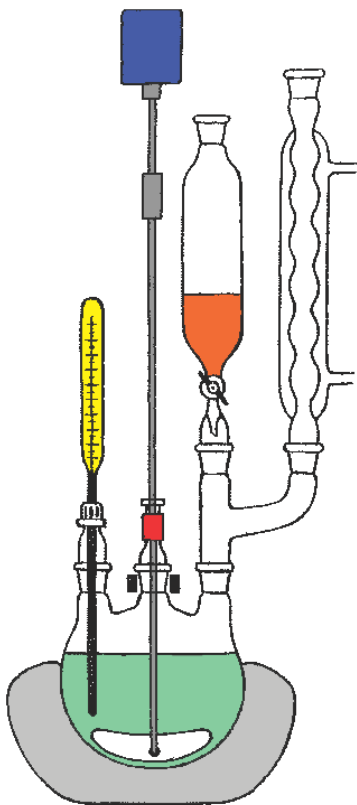
DHA Synthesis ... *Easy to do*



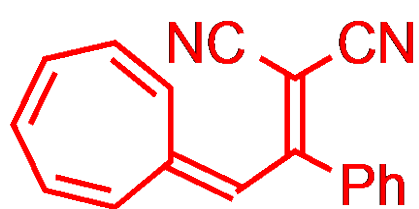
1) TrBF_4
 $\text{CH}_2\text{ClCH}_2\text{Cl}$
2) Et_3N , PhMe



optimized to 15 g scale

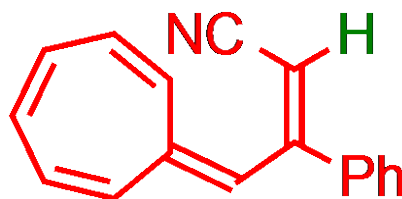


Energy Storage

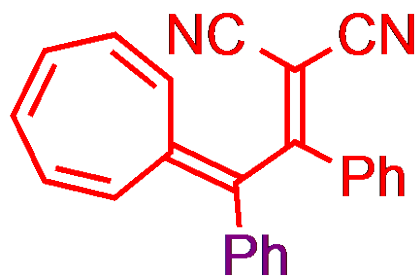


0.11 MJ / kg

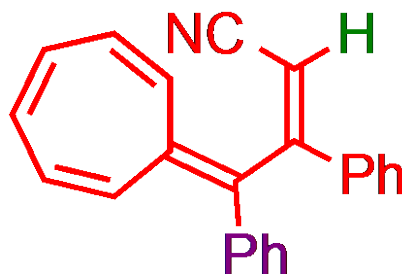
Substitute one
CN for a H



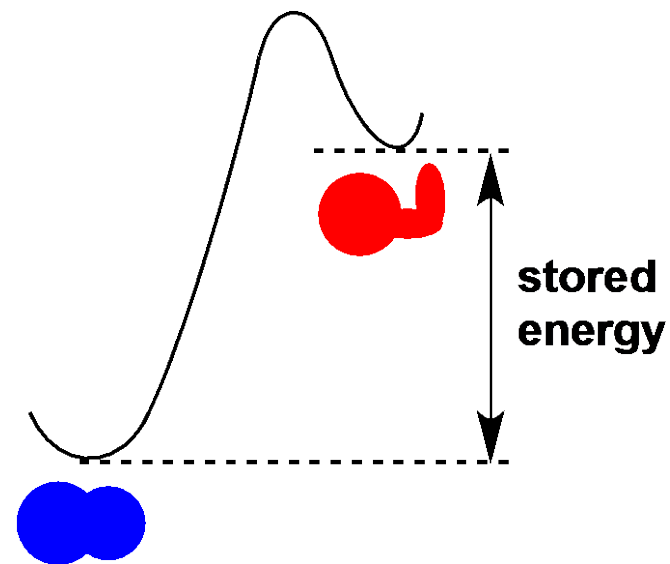
0.25 MJ / kg



0.15 MJ / kg



0.23 MJ / kg

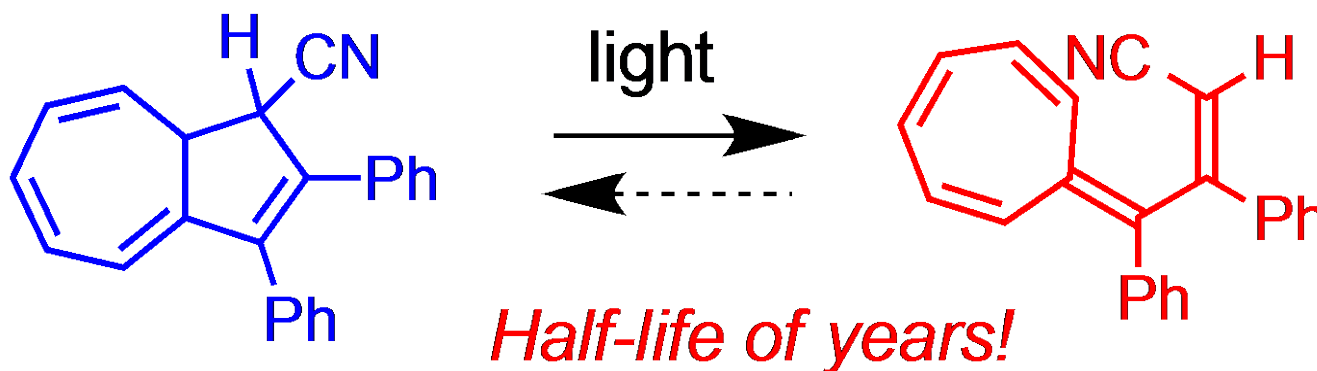
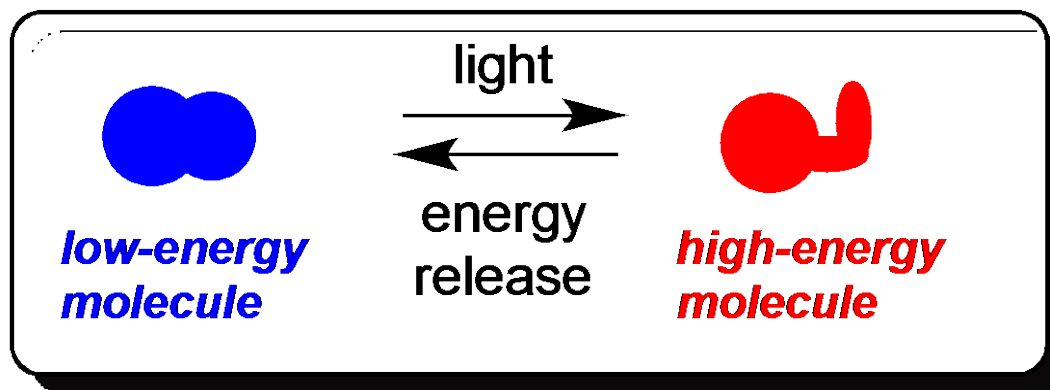


By minor structural variations we have recently doubled the energy density!

S.T. Olsen, J. Elm, F.E. Storm, A.N. Gejl, A.S. Hansen, M.H. Hansen, J.R. Nikolajsen, M.B. Nielsen, H.G. Kjaergaard, K.V. Mikkelsen, *J. Phys. Chem. A* **2015**, *119*, 896-904.

M. Cacciarini, A.B. Skov, M. Jevric, A.S. Hansen, J. Elm, H.G. Kjaergaard, K.V. Mikkelsen, M.B. Nielsen, *Chem. Eur. J.* **2015**, *21*, 7454-7461.

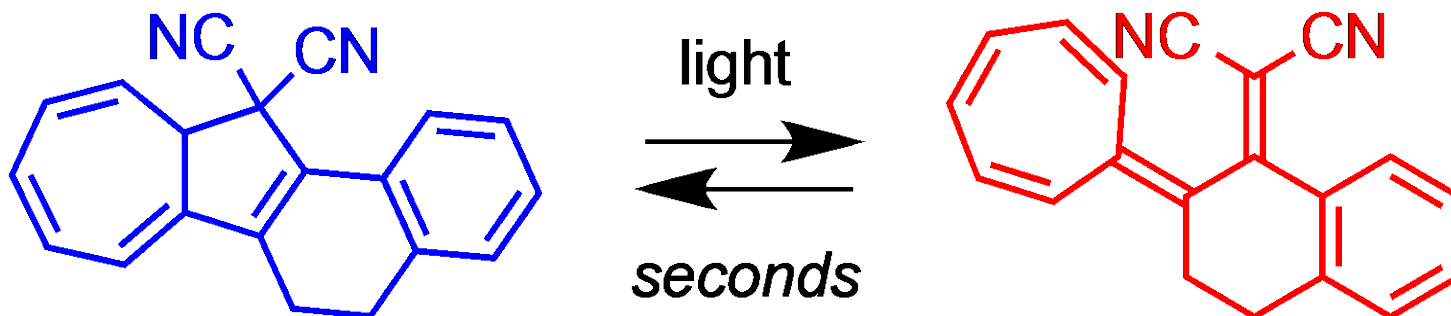
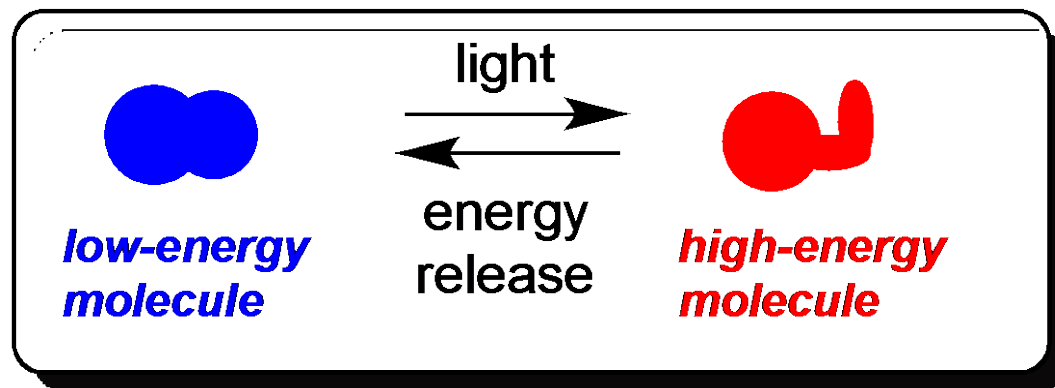
Halting the Energy-Releasing Back-Reaction



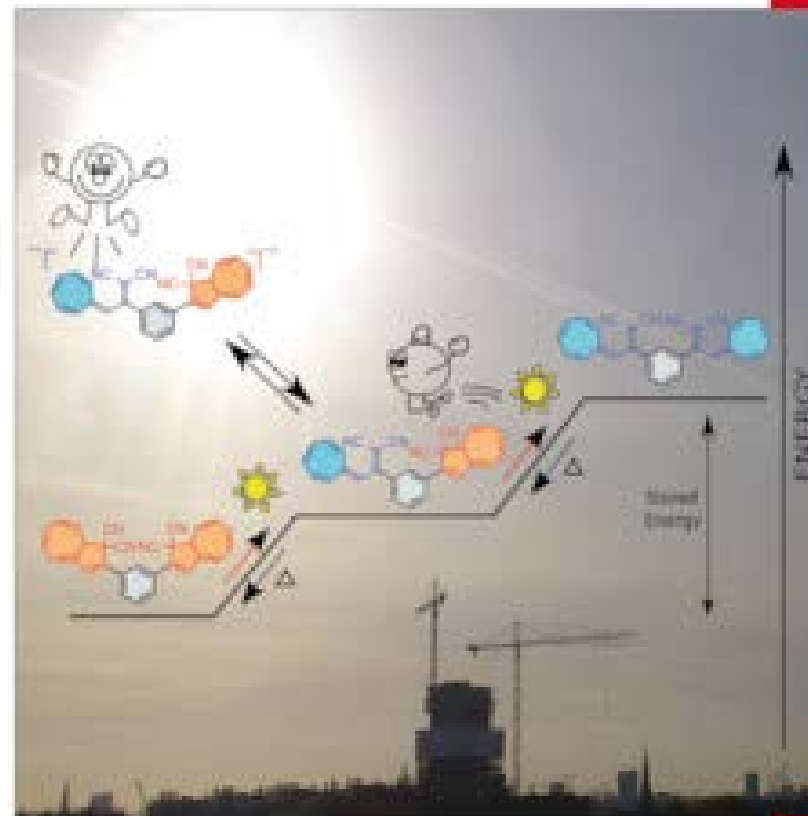
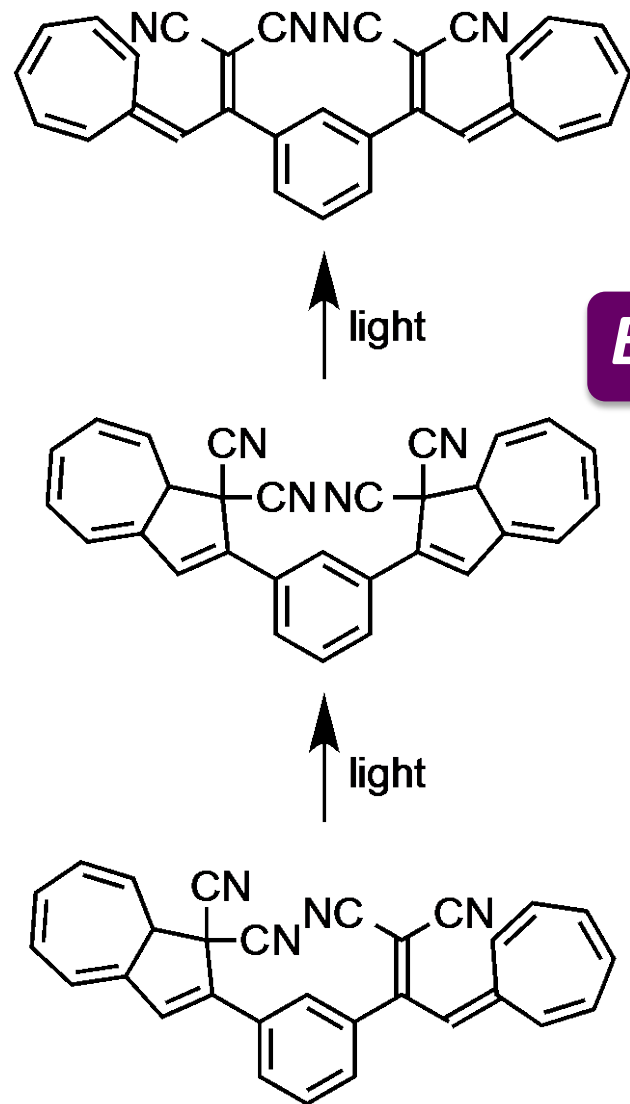
... We are currently working on triggering the energy release by a catalyst

The Other Extreme: A Very Fast Photoswitch

Light-Harvesting followed by Immediate Energy Release



Molecules with Two or More Photochromic Units

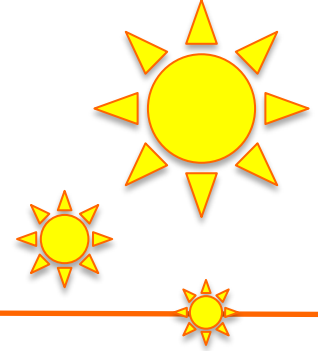


Two dihydroazulene photoswitches ...

... operated by a microfluidic device can be spatially controlled to investigate microfluidic systems under the influence of light at the intermediate species, representing reduced photoactivity due to a charge-transfer quenching mechanism. Obviously, both dihydroazulene units are fixed to the high-energy vinylphthalazine moieties, where the energy is temporarily stored. For more details, see the Full Paper by M. Simionescu-Nikolic et al. on page 3969.



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Department of Chemistry, University of Copenhagen***



Thank you!