Q-CHEM

A QUANTUM LEAP INTO THE FUTURE OF CHEMISTRY

Study of excited states

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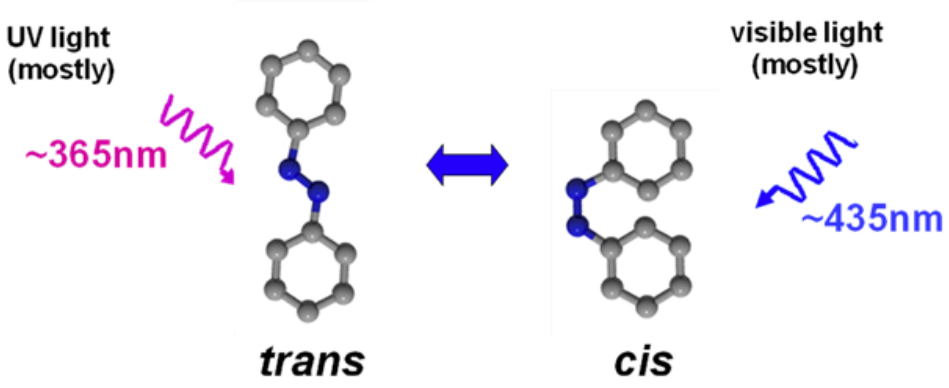
Q-Chem User Workshop, Munich

August 26, 2017

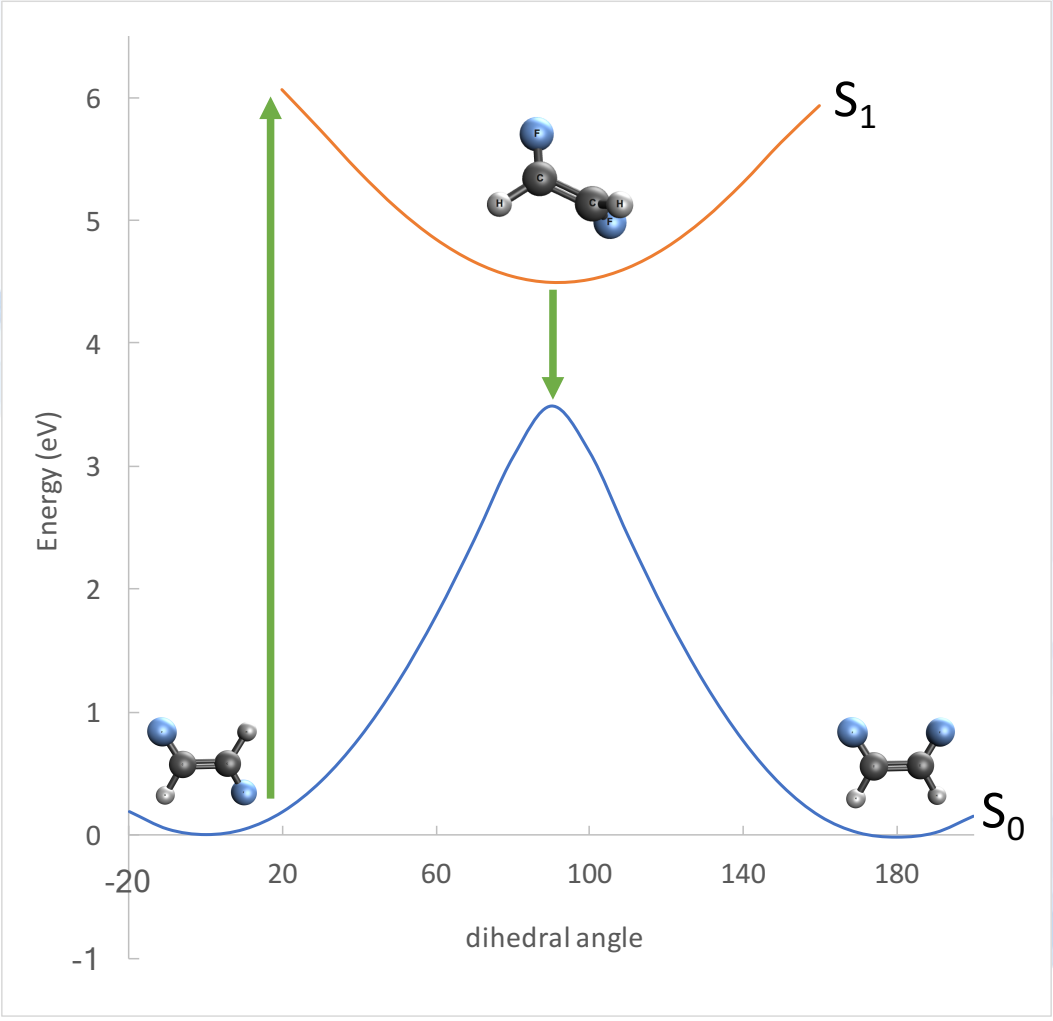
Azobenzene and Its Derivatives



Azobenzene is an incredible small organic molecule that has the potential to perform as a photoswitchable nanoscale piston on a surface. Azobenzene exists in two different shapes (isomers, labeled *trans* and *cis*) and can be reversibly and reliably driven between these two shapes by shining UV and blue light on it (photoisomerization). The lengthening and contracting of azobenzene as it changes shape allows it to do mechanical work.

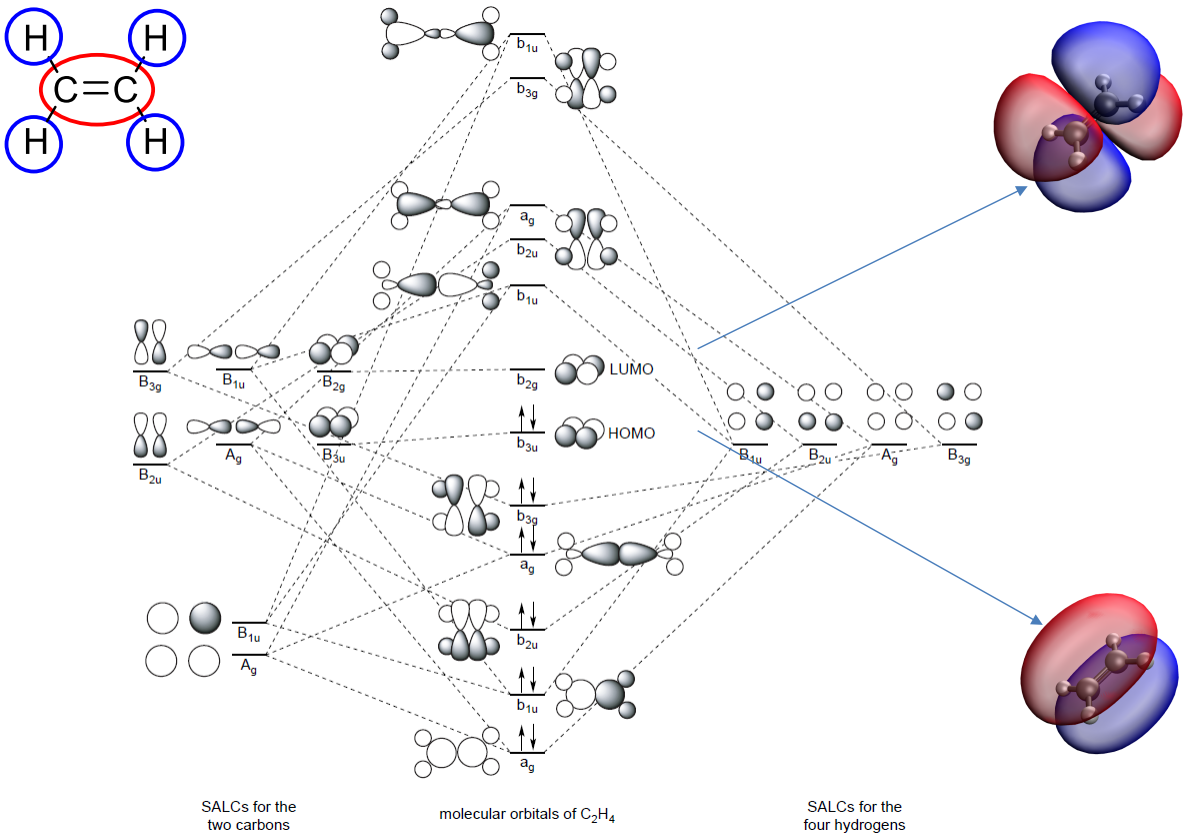
Source: http://research.physics.berkeley.edu/crommie/research:molecular-machines

Electronic states



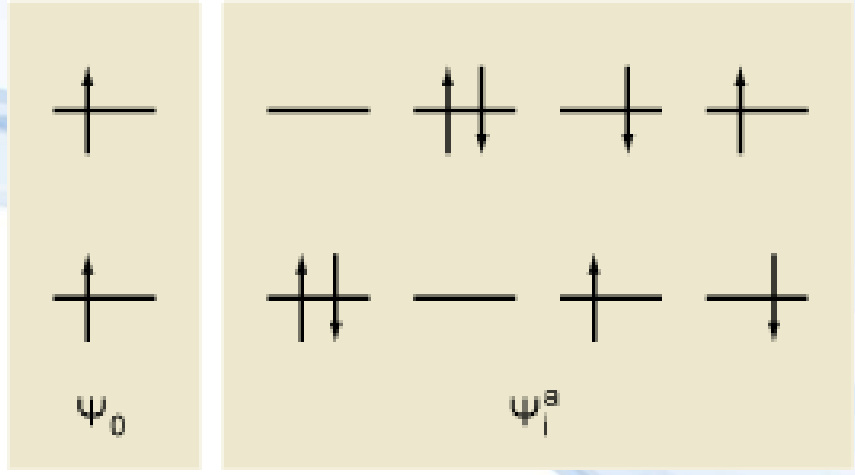
Ethylene MO diagram

Ethene Orbital Diagram



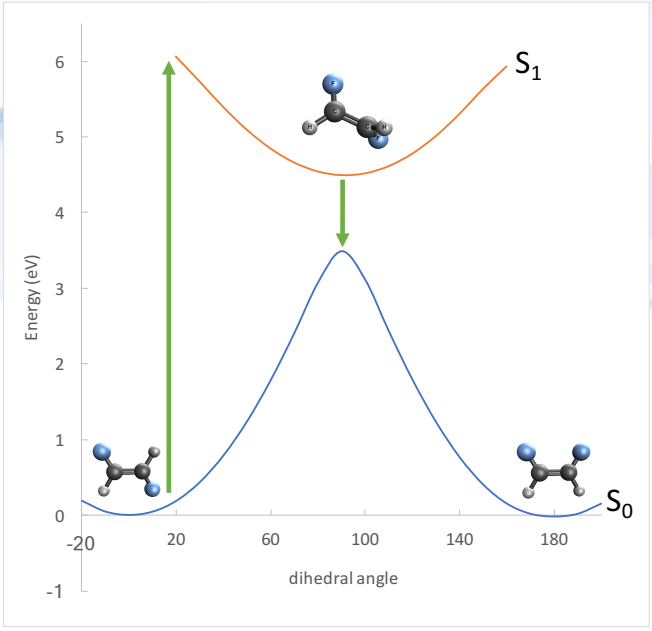
Spin-flip method

The spin-flip method enables the description of bond breaking through a single-reference formalism.



Spin-flip is available for TD-DFT, EOM, ADC methods.
RAS-*n*SF describes multiple bond breaking.

Photoisomerization of $C_2H_2F_2$



- Evaluate the excitation energy at the ground state equilibrium
- Locate the minimum energy point on the excited state surface
- Evaluate the excitation energy at the excited state equilibrium