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### Why studying photochromic molecules?

Photochromism is a reversible transformation of a chemical species induced in one or both directions by absorption of electromagnetic radiation between two form, A and B, having different absorption spectra, or more generally different physical properties, also other than spectroscopic (optical) ones. [1] Dealing with systems having so two stable isomers and the possibility to go from one isomer to other simply by irradiation, it is obvious to think about their possible application into optoelectronic devices, like optical memories, optical switches and display. [2,3]

Designing photochromic materials with improved optoelectronic properties necessarily needs a sound knowledge of the dynamics of the photoreaction they can undergo. For example, a fast reaction rate is desirable to get high reaction yield and high efficiency in optoelectronic devices. Furthermore, a high quantum yield is usually coupled with a reduction of unwanted side-reactions and so with an improved fatigue resistance. [4,5]

One of the biggest obstacles to the use of these systems is that technical applications usually require their dispersion into solid matrices, e.g. polymeric matrices, nanoobjects, ... : in this case, also a photochromic activity suppression has been reported. [2] A first step to characterize the effect of the neighbourhood on the excited state dynamics can be the introduction of these systems in a controlled environment, like an Ar<sub>n</sub> cluster or nanoparticles.

[1] Bouas-Laurent, H.; Durr, H., *Pur. Appl. Chem.* **2001**, *73*, 639

[2] Irie, M., *Chem. Rev.* **2000**, *100*, 1685

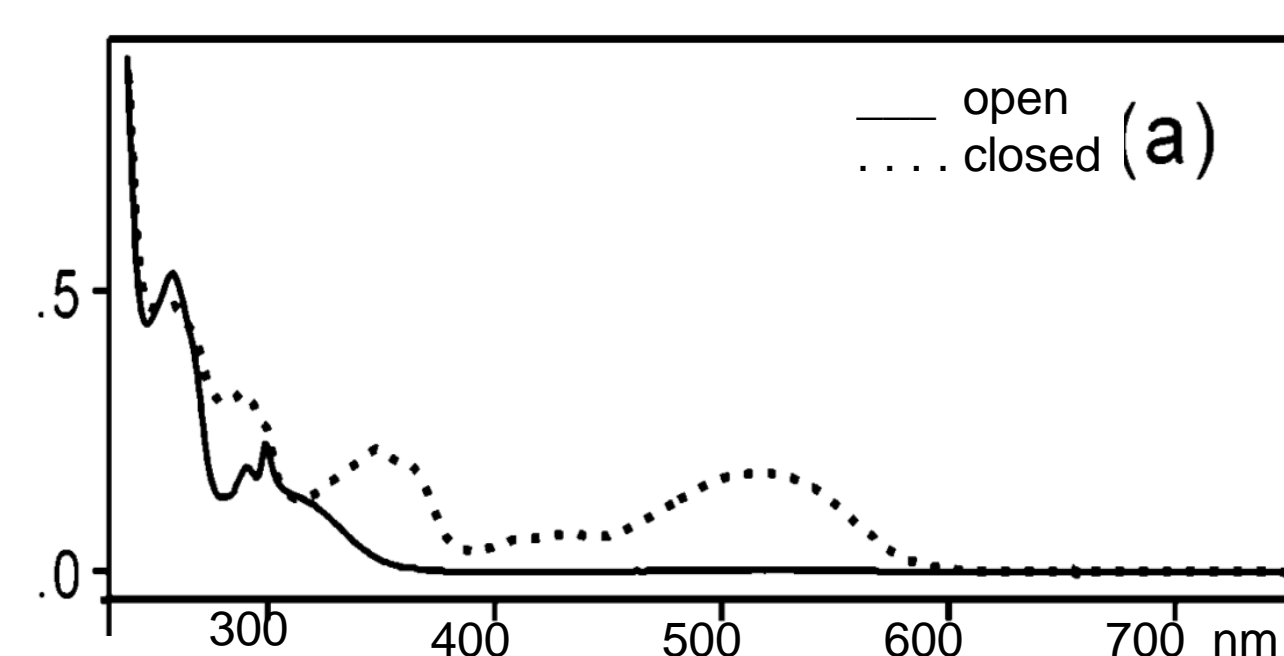
[3] Tamai, N.; Miyasaka, H.,

*Chem. Rev.* **2000**, *100*, 1875

[4] Shim, S.; Eom, I.; Joo, T.; Kim, E.;

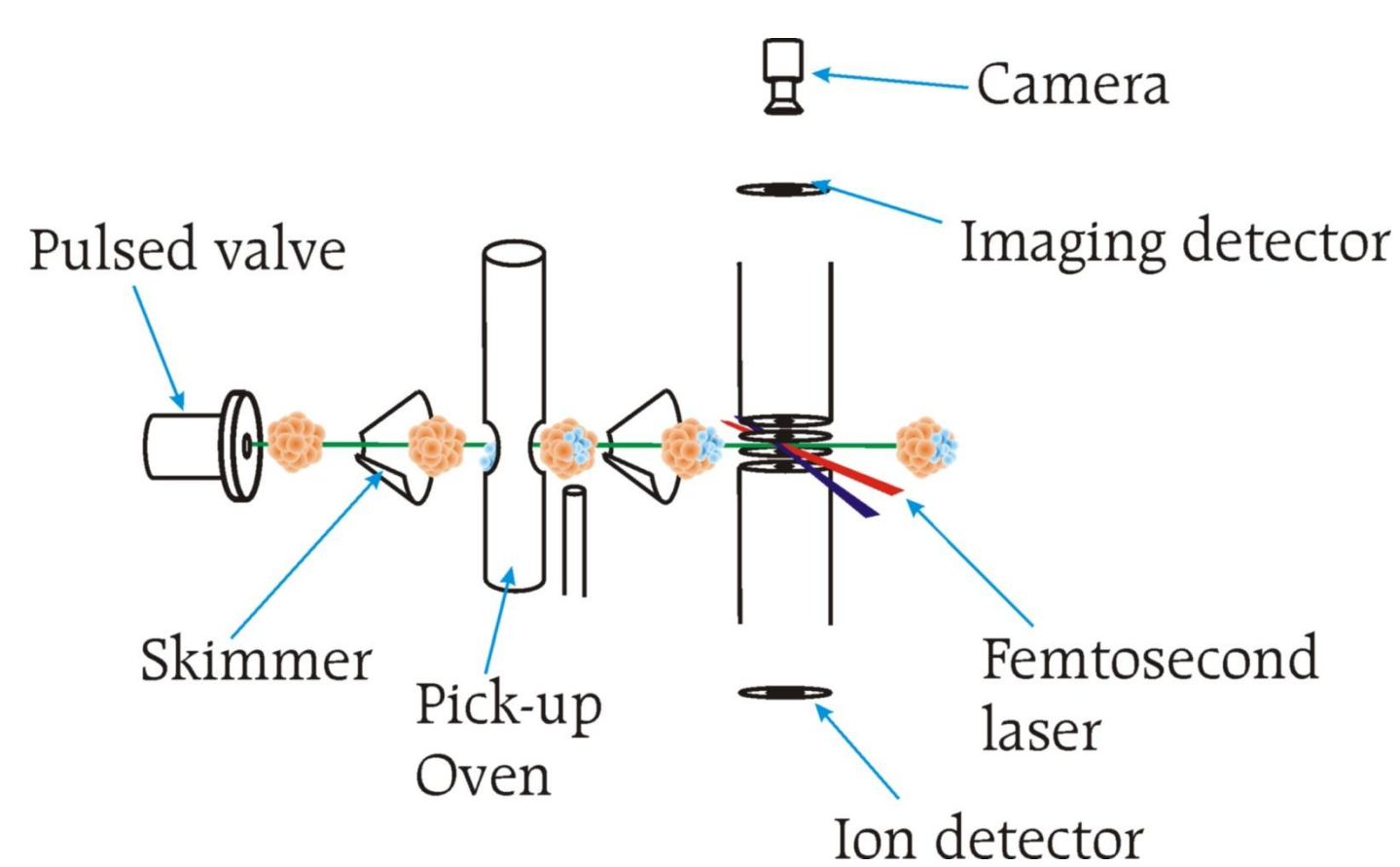
Kim K. S., *J. Phys. Chem. A* **2007**, *111*, 8910

[5] Y. Ishibashi, et al., *J. Phys. Chem. C*,  
**2011**, *115*, 4265–4272.



Absorption spectra (in solution) for open and closed BTF6 isomers (adapted from ref.[4])

### Reaction dynamics of the deposited molecule

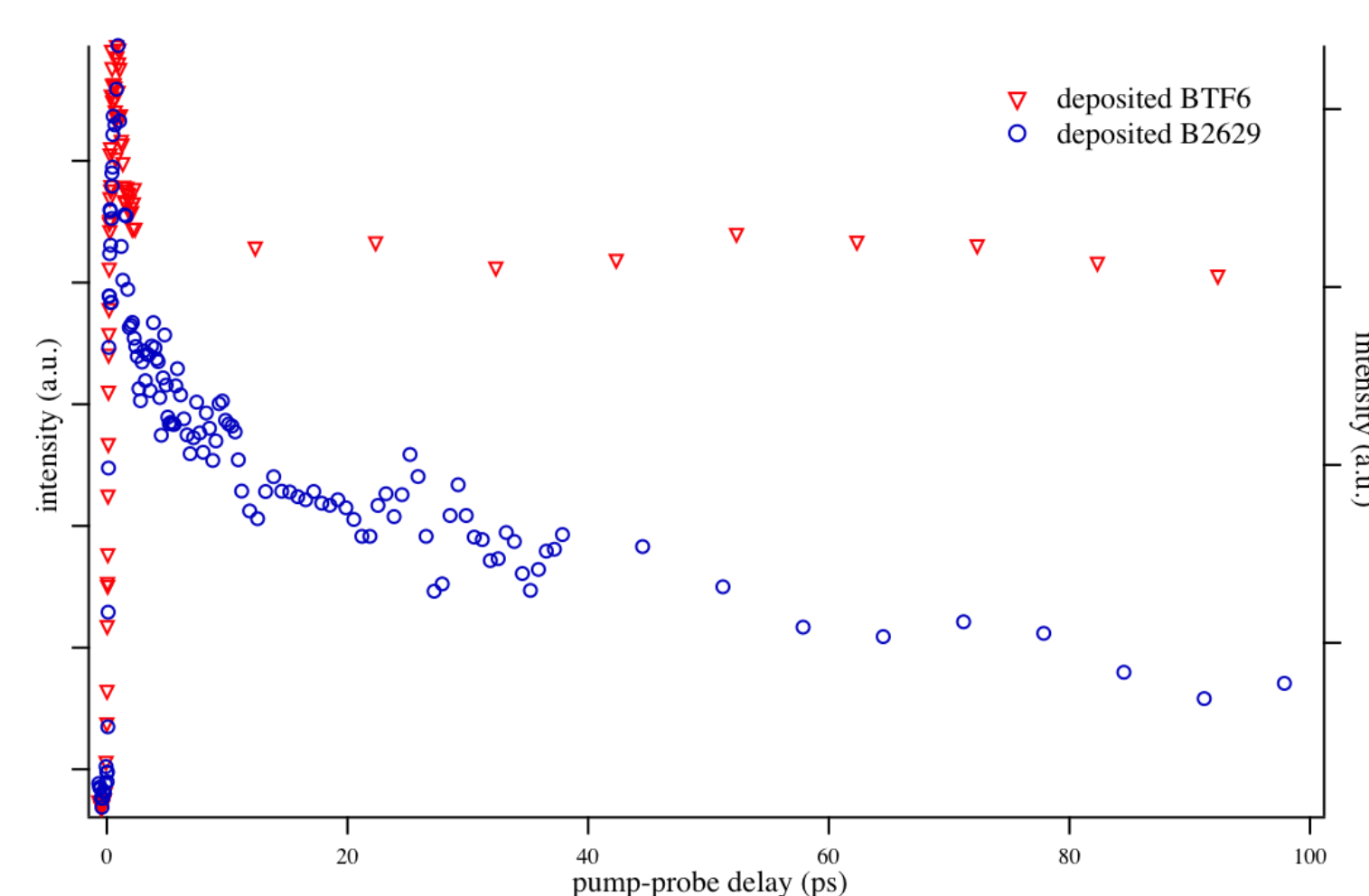


The molecules are deposited on argon cluster, which is a model of solvating medium as its temperature is 34K, it is chemically inert and interact only by polarization.

The reaction dynamics observed is different since, depending on the molecule, some process are blocked.

This is interpreted by a difference in the part of the potential energy surface that is explored due to the 1/ Initial temperature 2/ Initial geometry 3/ Vibrational cooling down process by the medium during the relaxation process.

Calculations are in progress to elucidate the initial geometry of the solvated molecule.



### Scientific production

M. Sliwa, N. Mouton, C. Ruckebush, L. Poisson, A. Idrissi, S. Aloïse, L. Potier, J. Dubois, O. Poizat, G. Buntinx, *Photochem. Photobiol. Sci.*, **9**, 661-669 (2010)

S. Aloïse, Z. Pawlowska, C. Ruckebush, M. Sliwa, J. Dubois, O. Poizat, G. Buntinx, A. Perrier, F. Maurel, P. Jacques, J.-P. Malval, L. Poisson, G. Piani, J. Abe, *PCCP*, **14**, 1945–1956 (2012)

J. Köhler, P. Hemberger, I. Fischer, G. Piani, and L. Poisson « Ultrafast Dynamics of Isolated Fluorenone », *J. Phys. Chem. A*, **115** (50), 14249–14253 (2011)

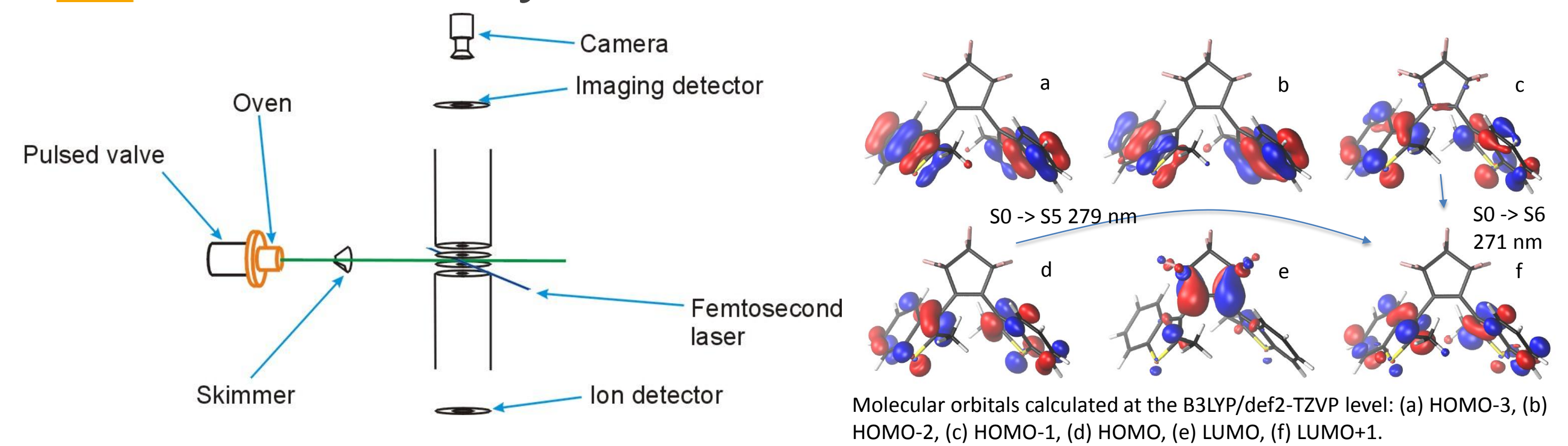
P. Hemberger, J. Köhler, I. Fischer, G. Piani, L. Poisson and J.-M. Mestdagh « Femtosecond Dynamics of Cyclopropenylidene, c-C3H2 », *PCCP*, **14**, 6173–6178 (2012),

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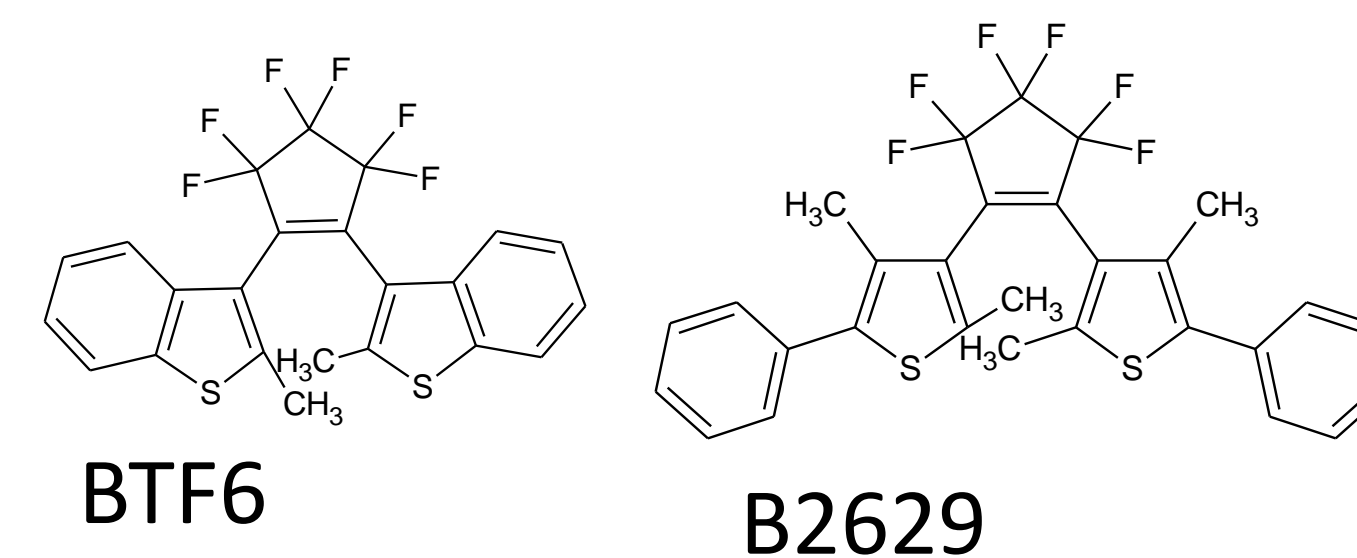


### Reaction dynamics of isolated molecule



Pump laser = 266 nm

Probe laser = 800 nm



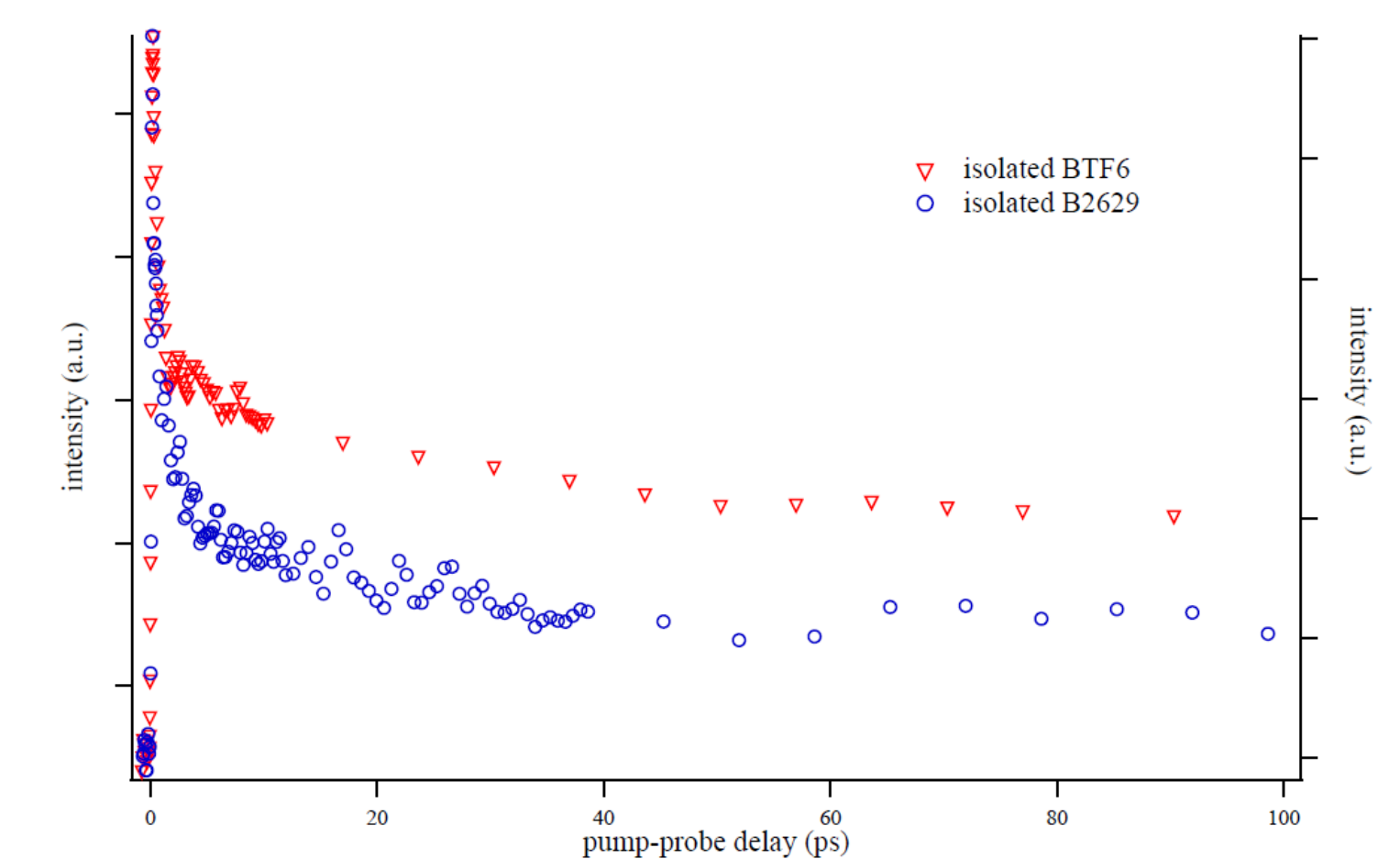
Diarylethenes

The time resolved ring closure of several diarylethene (two of them presented here) was monitored using the pump/probe method with a ~50 fs time resolution.

3 time scales are usually observed:

B2629	250 fs	6ps	100 ps
BTF6	600 fs	X	60 ps

Attributed to 1/ Direct relaxation to the ground state through a Conical intersection  
2/ Vibronic relaxation to the ground state 3 / Relaxation of isomers



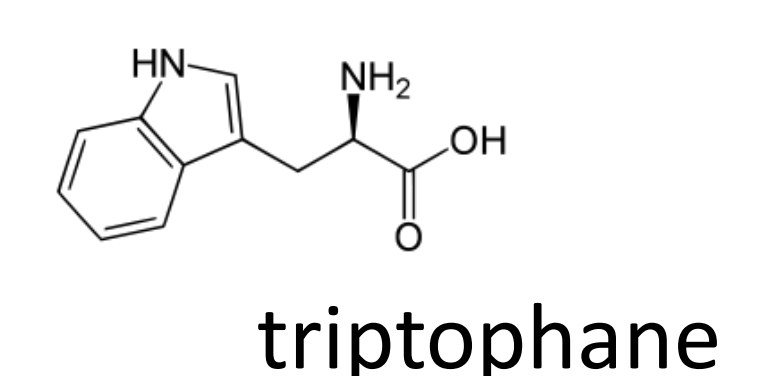
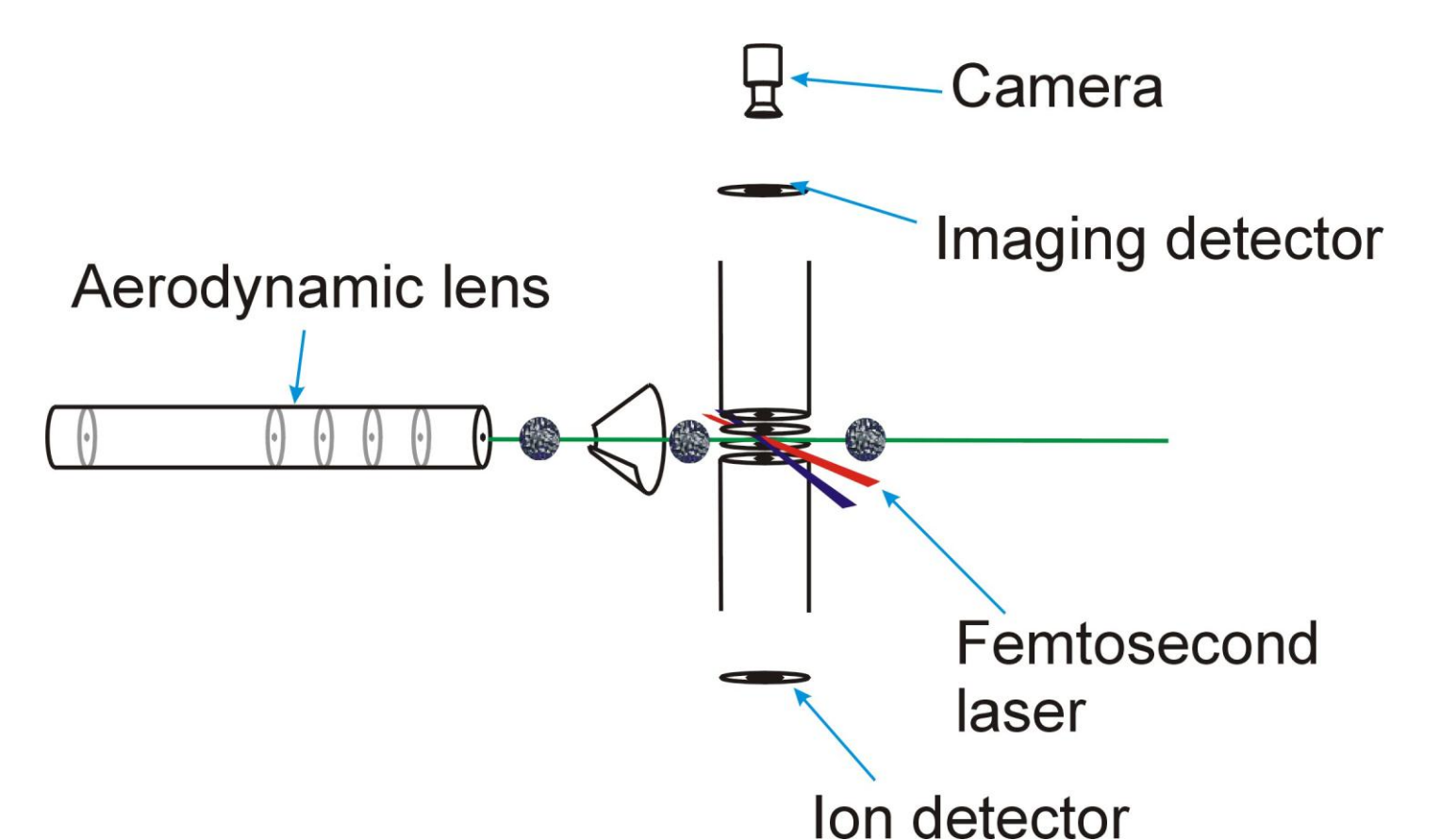
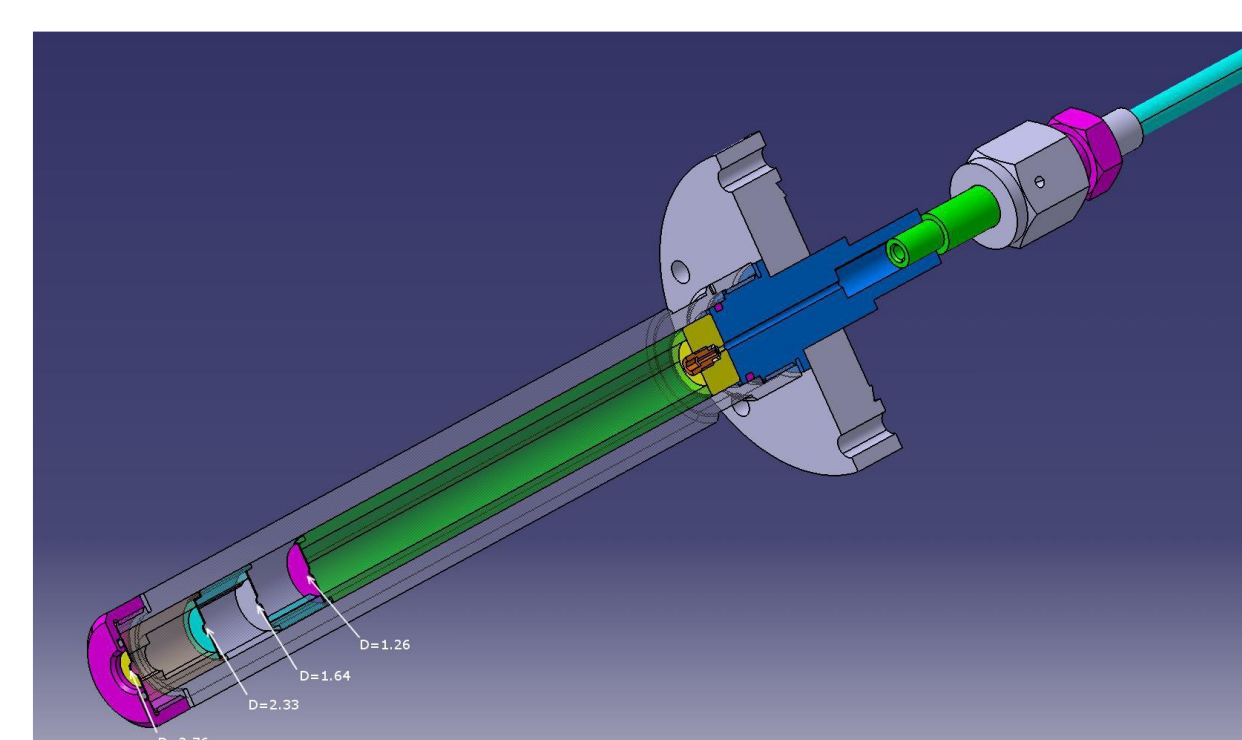
### Characterization of nanoparticle beam

The next step consists in the study of nanoparticles of photochromic molecules and of deposited photochromic molecule on well defined nanoparticles.

This will be performed through a collaboration with

- the SOLEIL synchrotron facility : beamline PLEIADES (PNANO / NANO-PLIEADES) and beamline DESIRS (Collaboration with François GAIE-LEVEL)
- ISMO laboratory (Satchin SOORKIA)

A first test has been performed in our experiment using the aerodynamic lens built by the beamline DESIRS from SOLEIL. Nanoparticles of tryptophane were observed upon strong irradiation.



Based on this test, we designed and built a new aerodynamic lens devoted to small nanoparticles. It is currently under test on SiO<sub>2</sub> nanoparticles.

X. Wang, P. H. McMurtry, *Int. J. Mass Spectrom.* **2006**, *258*, 30-36.