Dipartimento di Chimica Industriale
"Toso Montanari"

CHIMICA FISICA DEI MATERIALI FUNZIONALI

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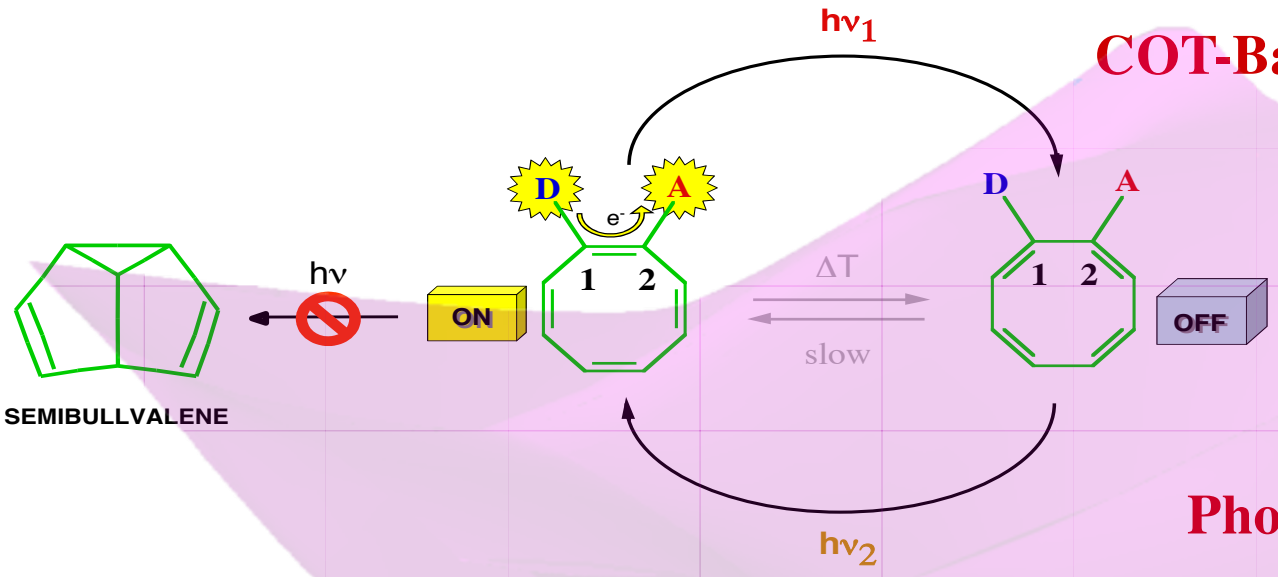
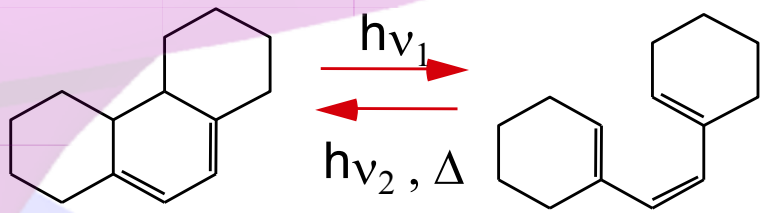
COT-Based Photochemically Driven Switch



Angew, 2001, 40, 1466
JACS, 2002, 124, 13770

Photochromic Compounds

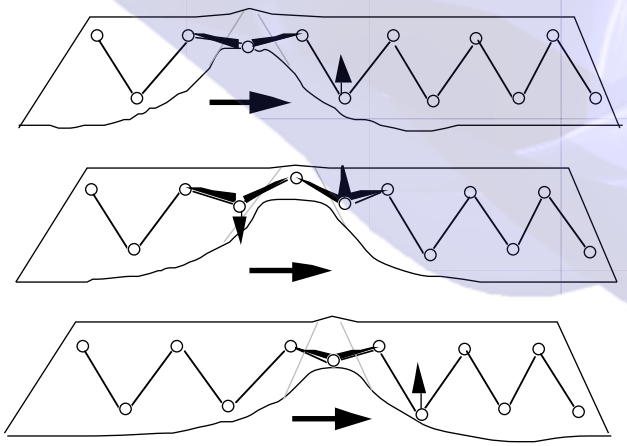
X = O, S



JPC-A, 2001, 105, 4458
JPC-A, 2003, 107, 11139; JACS 2008, 130, 7286

Photoconductivity: soliton motion

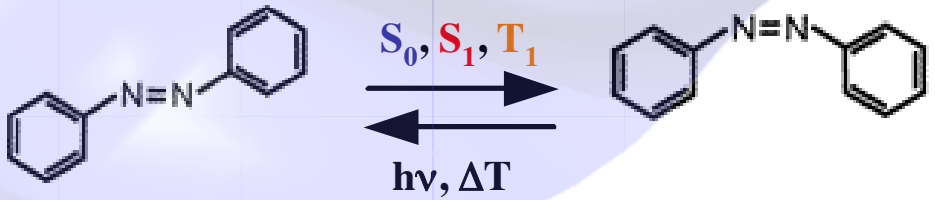
JACS, 2000, 122, 5568



Soliton motion

Azobenzene Photochemistry

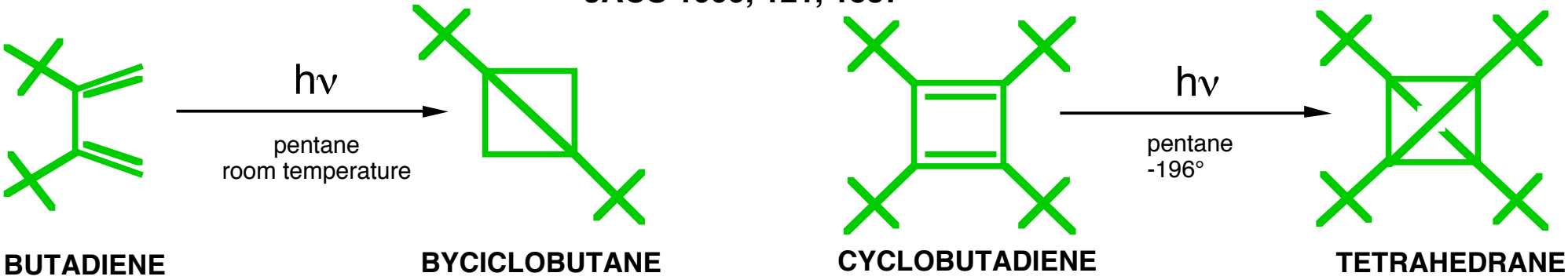
TCA, 2004, 111, 363
JACS, 2004, 126, 3234
JACS, 2007, 129, 3198; JACS, 2008, 130, 5216



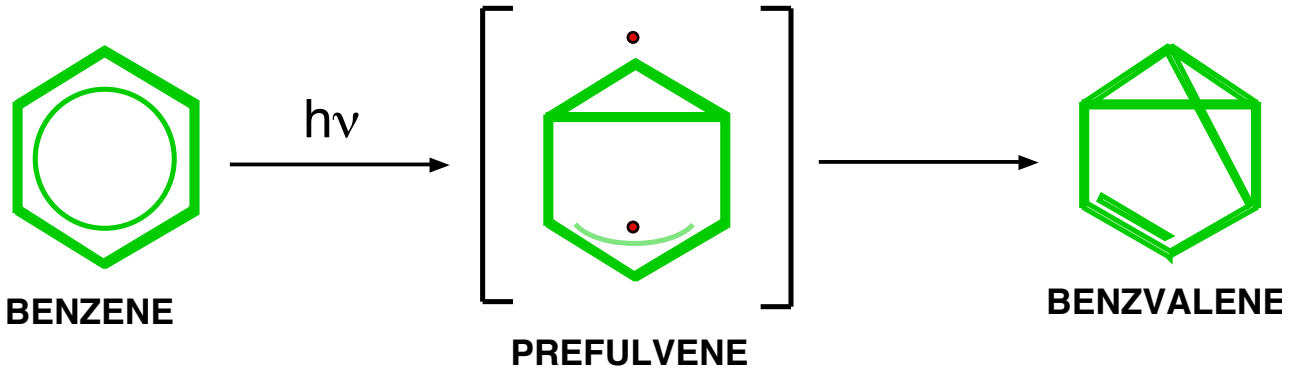
trans-azobenzene *cis*-azobenzene

Photoinduced Polycyclizations

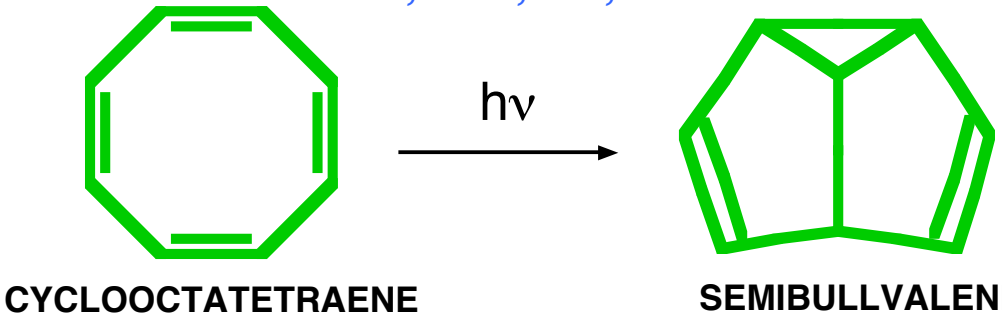
JACS 1999, 121, 1537



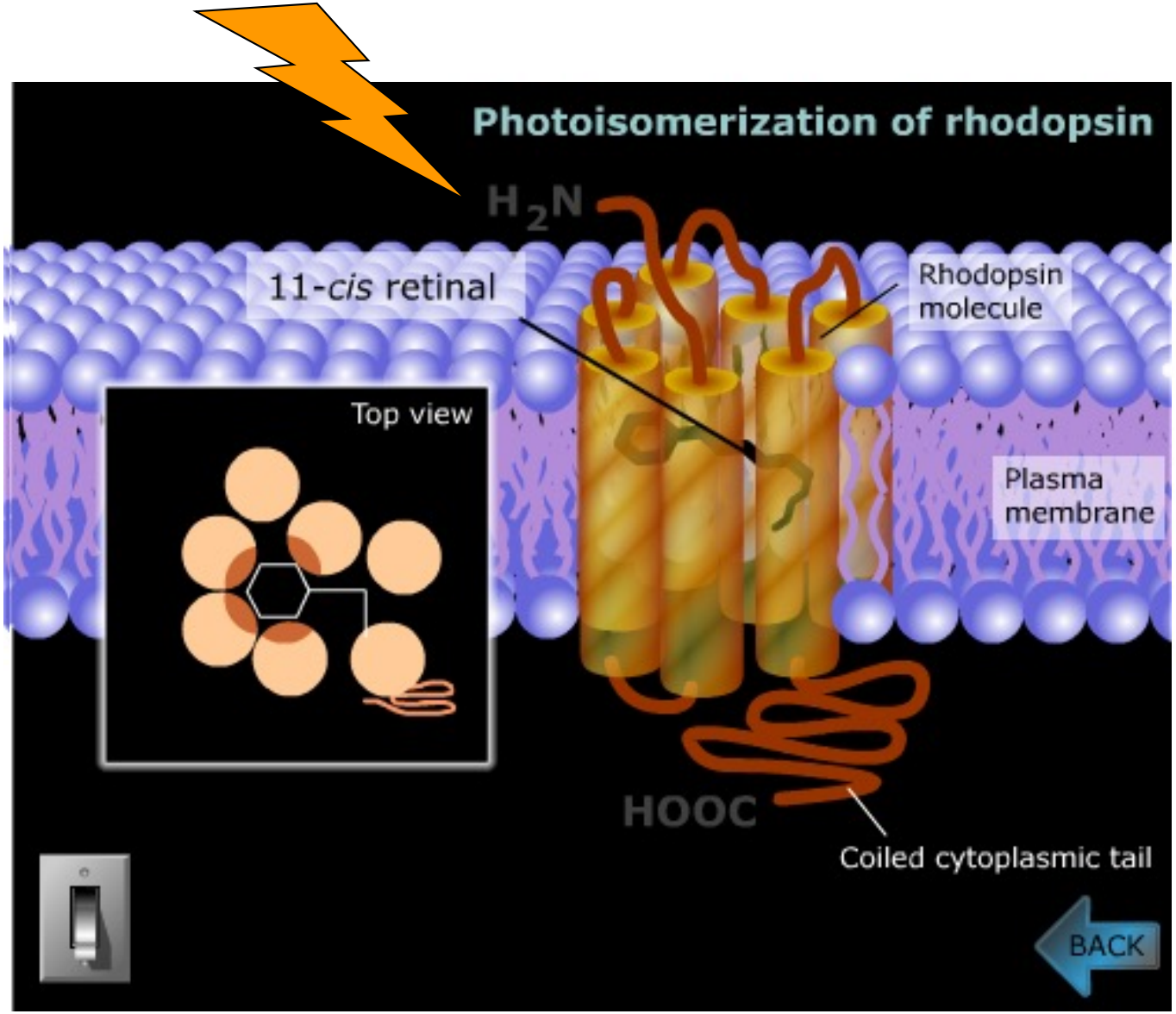
Rev. Comp. Chem. 2000, 15, 87



JACS, 2002, 124, 13770

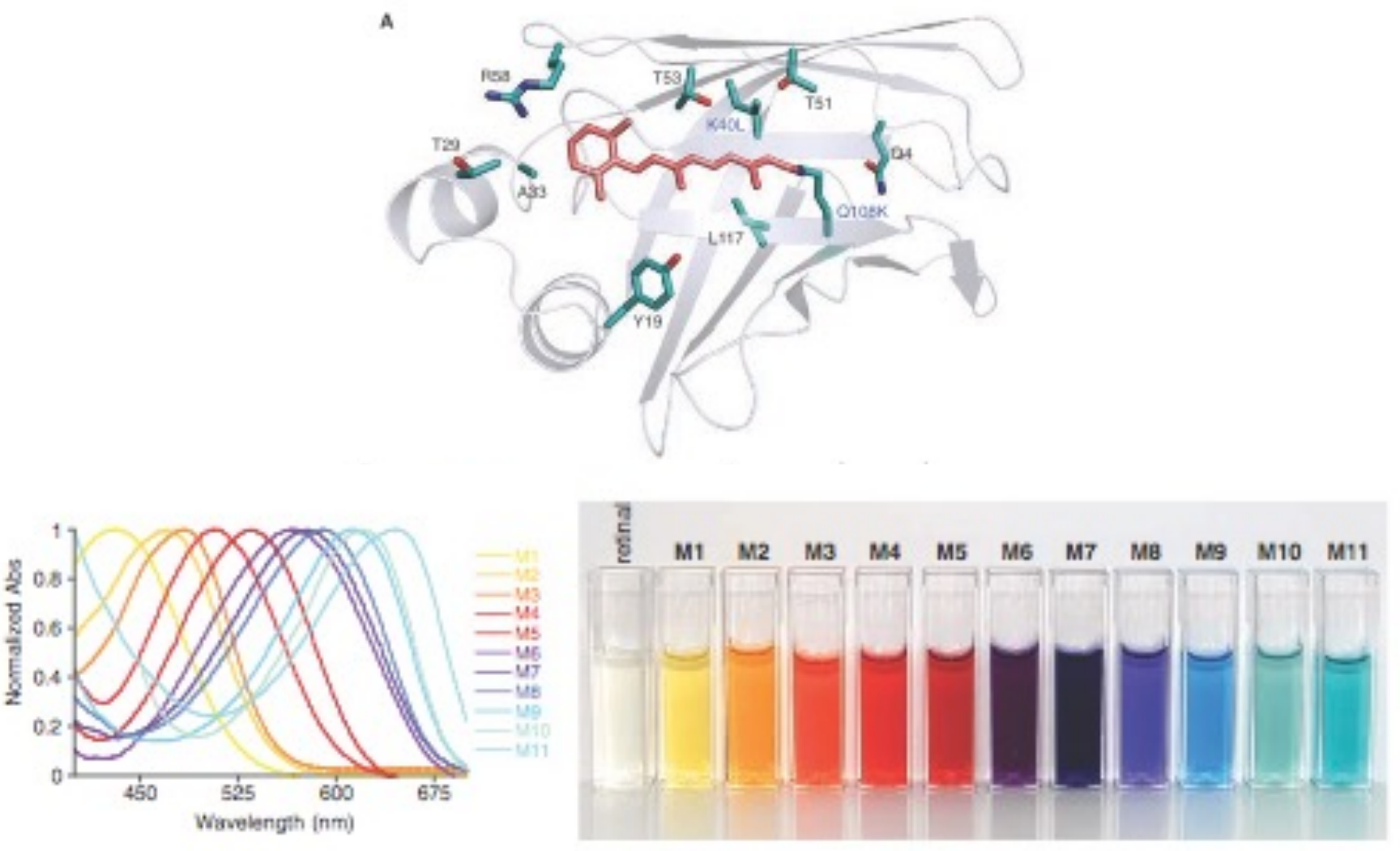


Ultrafast isomerization initiates vision



Re-engineering the retinal binding pocket

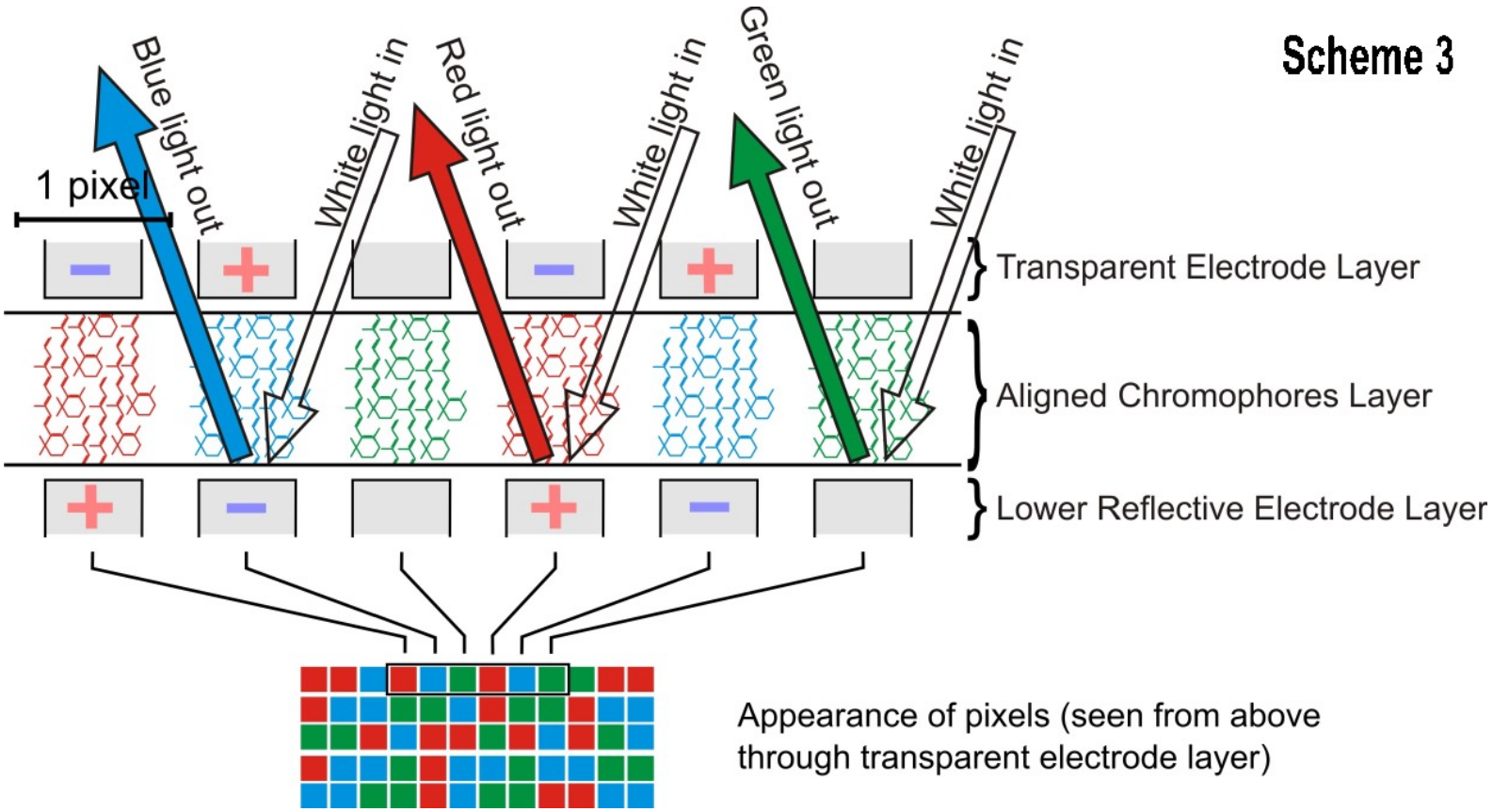
Rhodopsin mimics



Geiger and Borhan, *Science, 2012, 338, 1340-1343.*

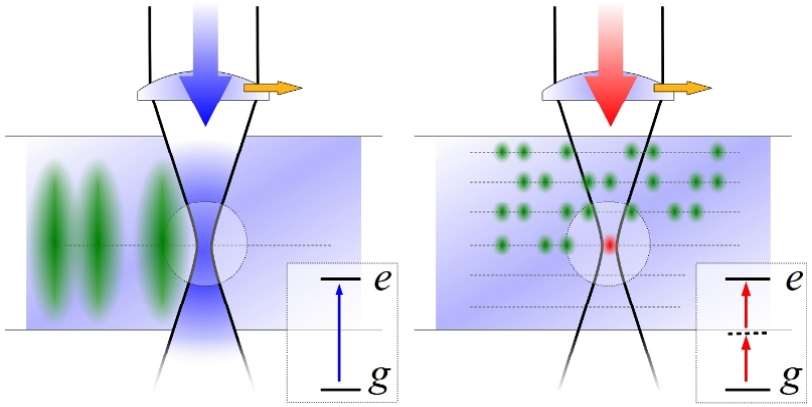
Electrochromism

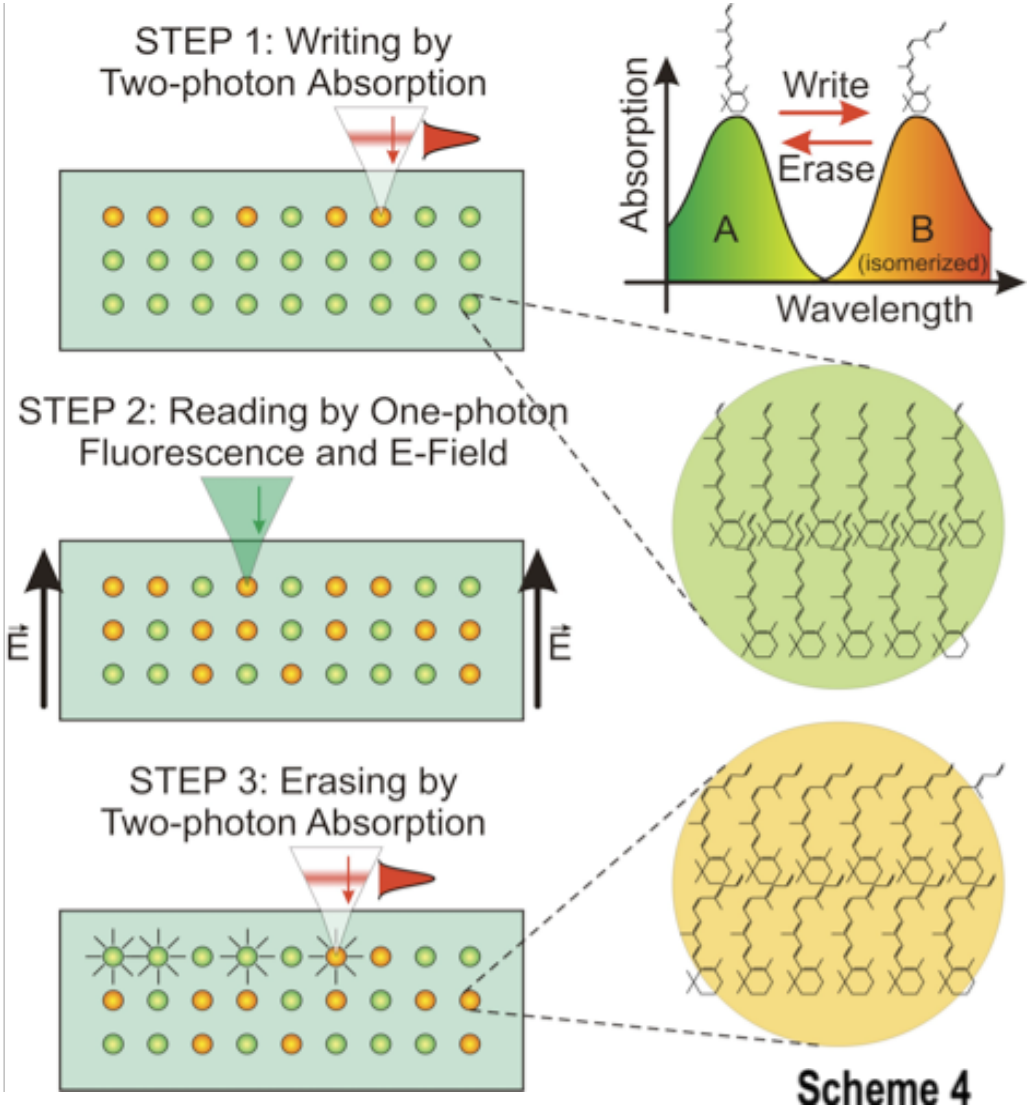
Full coloured/low-power consumption/high refresh-rate electronic-ink displays



Bio-inspired reversibly switchable fluorophores for **3D optical memories**

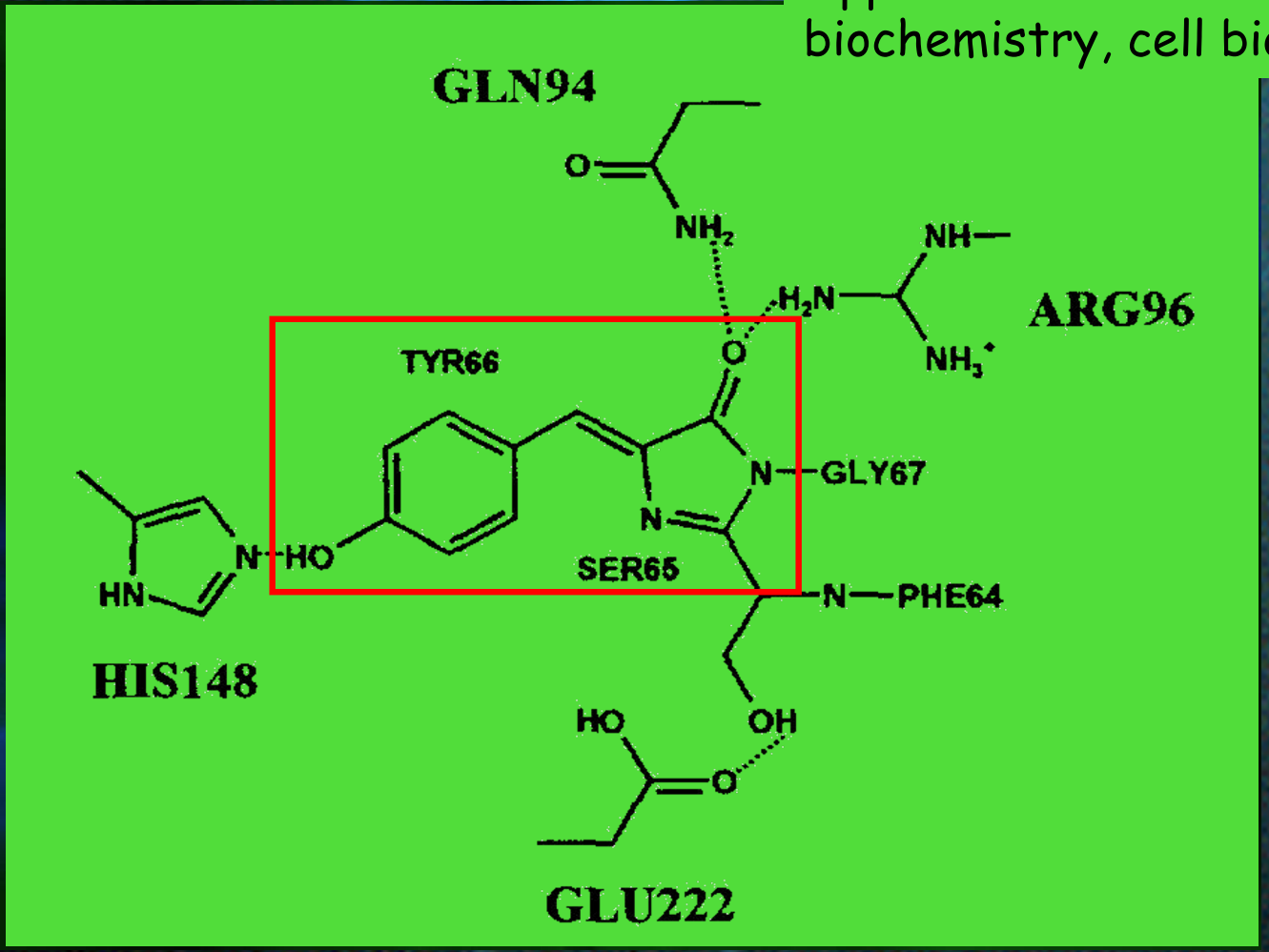
3D optical memories (by two-photon spectroscopy) based on reversibly switchable fluorescent systems





Fluorescent marker

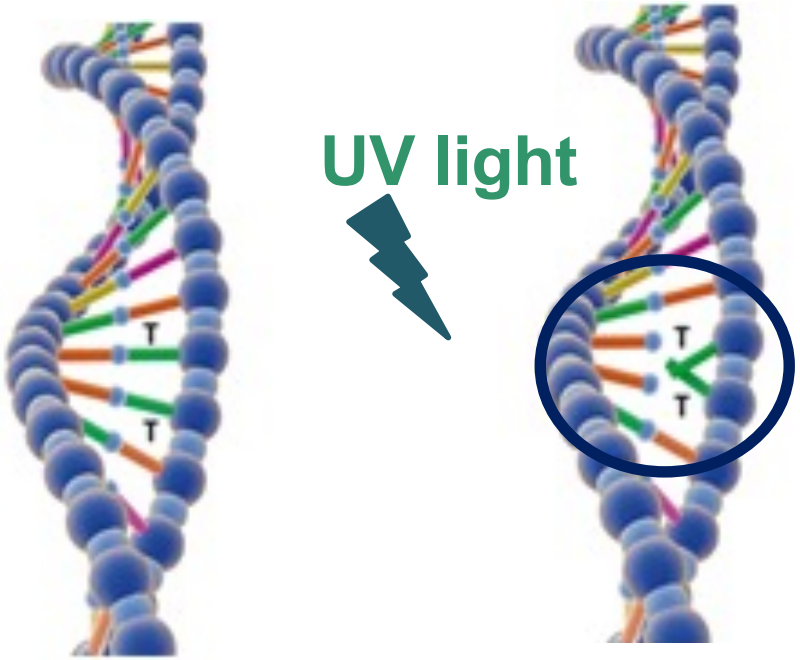
Applications in molecular genetics, biochemistry, cell biology



Aequorea victoria

Nucleic acids and UV light

UV light absorption might cause **damages** (formation of pyrimidine dimers, disruption in the strand, error during the copy and genomic lesions…)

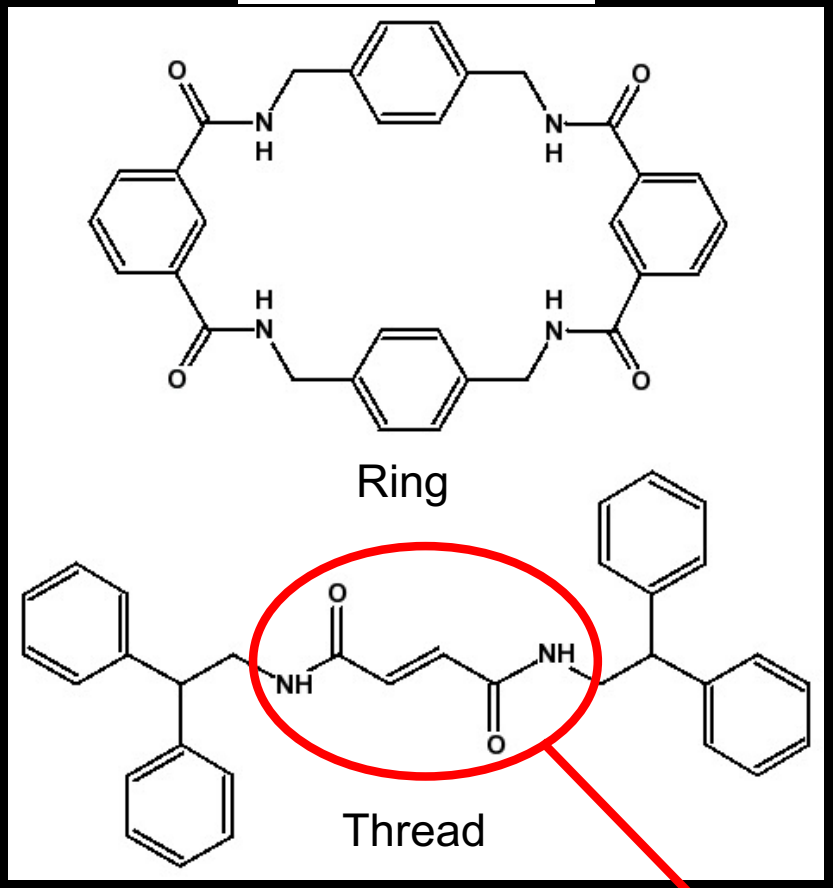


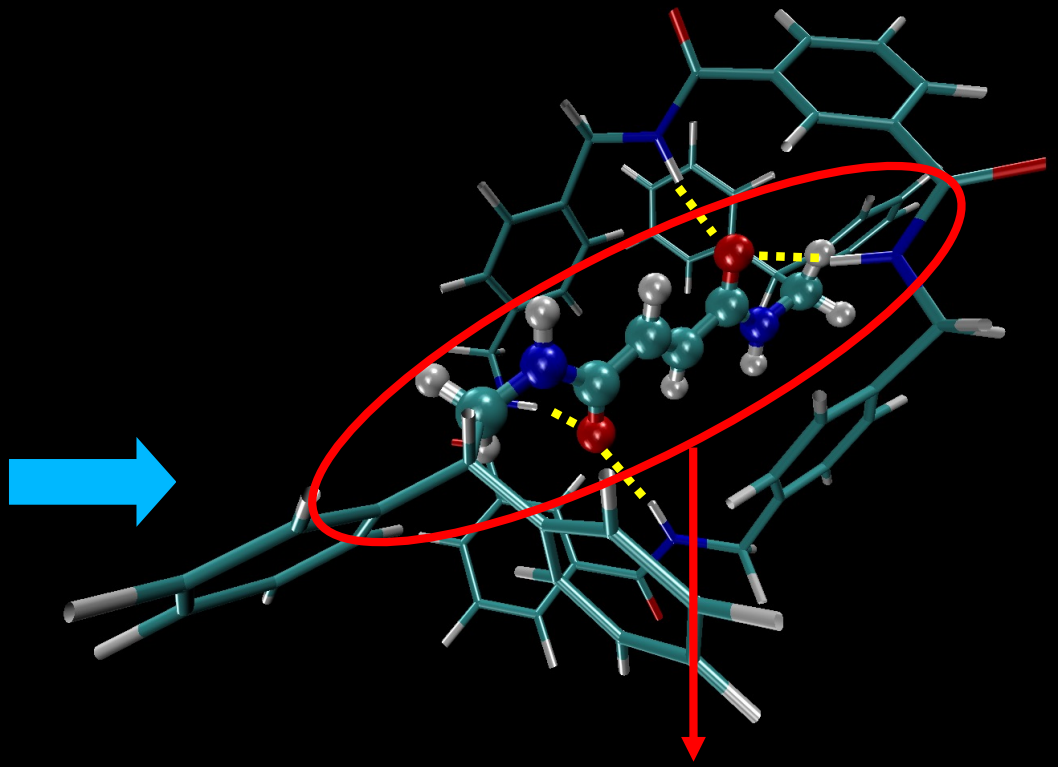
Canonical nucleobases have **photoprotective mechanisms** to prevent photochemical reactions: more than 99.9% of the photons are converted in a harmless way on the **ultrafast timescale**

Aim: understand ultrafast relaxation dynamics in DNA

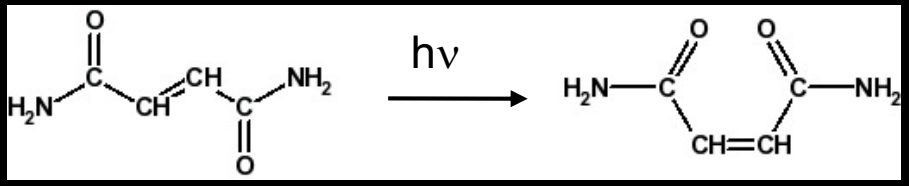
FUMARAMIDE BASED ROTAXANE: A PHOTOSWICHABLE SYSTEM

COMPONENTS





PHOTOACTIVE SYSTEM

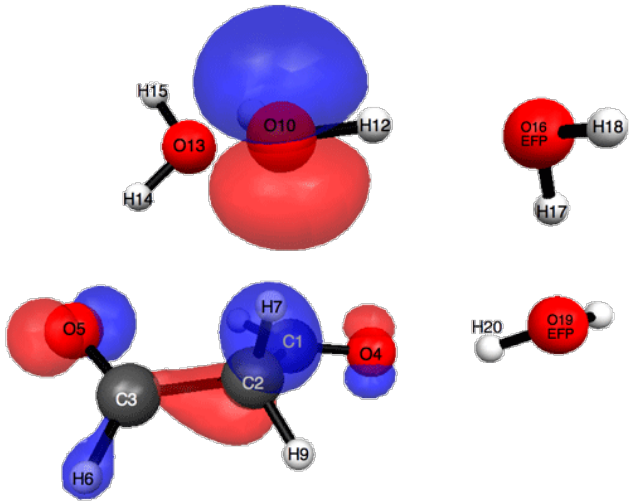


How to study a (photo)reaction mechanism within complex molecular systems?

Quantum Mechanical (QM) methods

$$H\Psi=E\Psi$$

Molecular properties are described by Quantum Mechanics which requires the solution of the Schrodinger equation



Only fundamental physical constants are required for *ab-initio* QM methods

QM methods can describe bond breaking and forming (electron coupling), excited states, decay

Systems larger than about 100/150 atoms cannot be studied

Molecular Mechanics (MM) methods

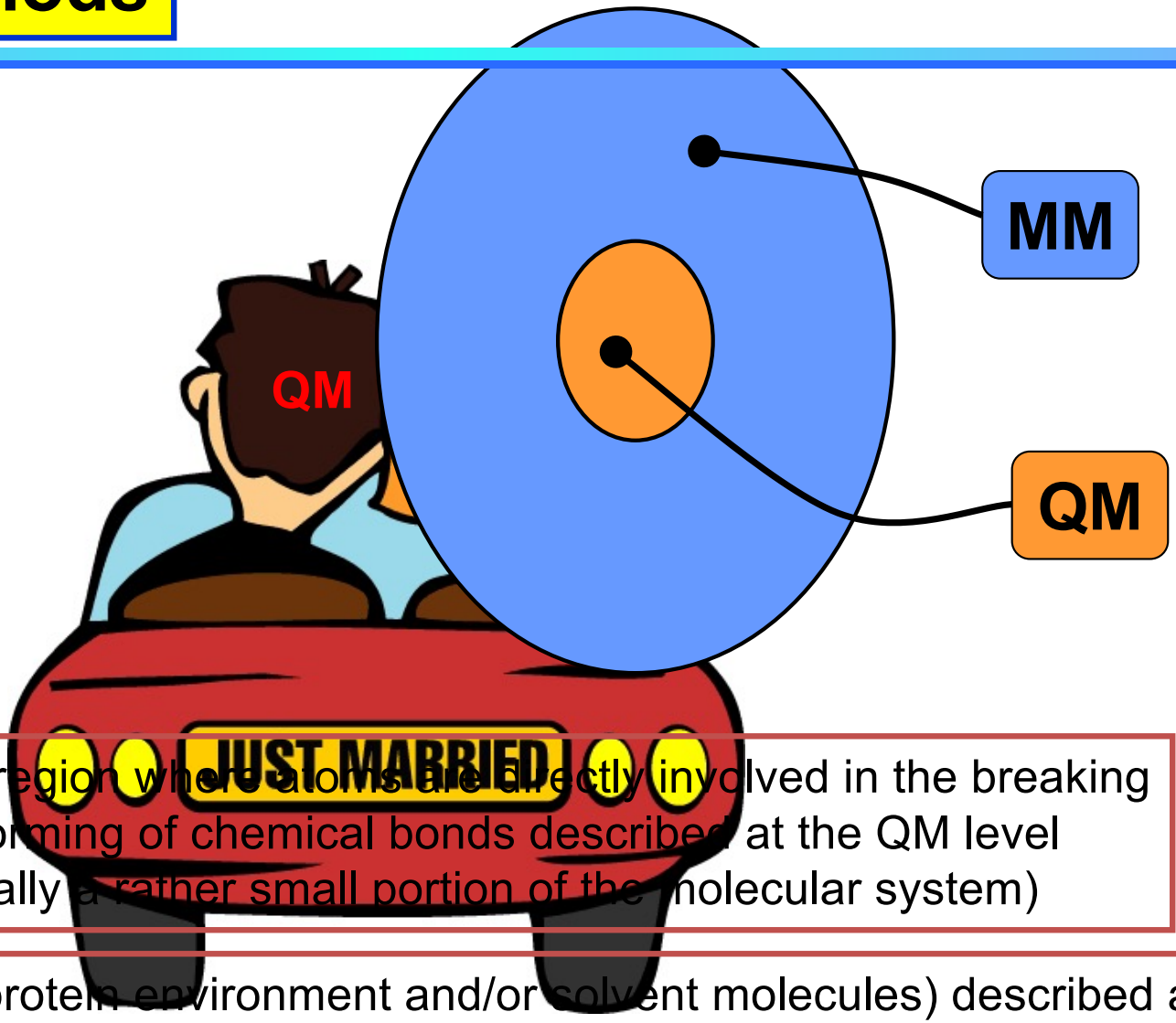
Based on classical physical laws (Newton's laws)
Atoms are simple spheres connected by springs (chemical bonds)
Point atomic charges are considered

Very fast, not expensive computations.
Accurate results for equilibrium structures and conformational problems

Electrons are not explicitely treated (they are only implicitely considered in the classical potentials)

Bond breaking and forming cannot be described
Excited states cannot be described
(Electronic problems cannot be described)

QM/MM Methods



Molecular region where atoms are directly involved in the breaking and forming of chemical bonds described at the QM level (usually a rather small portion of the molecular system)

Remaining atoms (protein environment and/or solvent molecules) described at the MM level (MM region is usually very large and can include many thousands of atoms)

The accuracy of the QM methods and the computational expedience of the MM approach are combined

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GRAZIE MILLE!

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