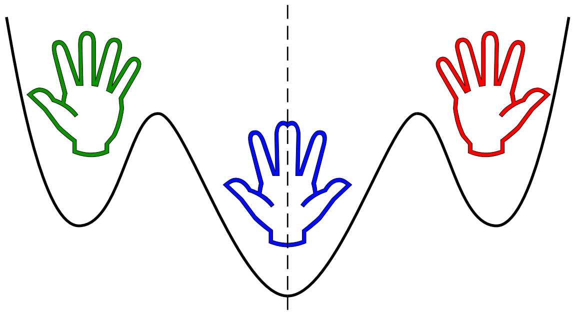
# Laser Induced Chirality
# &
# Enantiospecific Excitation

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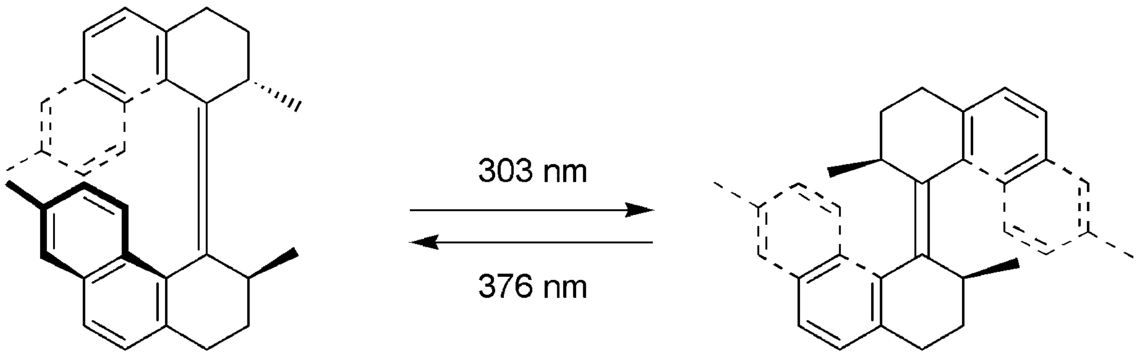
**Universität Potsdam**

# Chiroptical switch

## Photo-induced isomerization:[1]

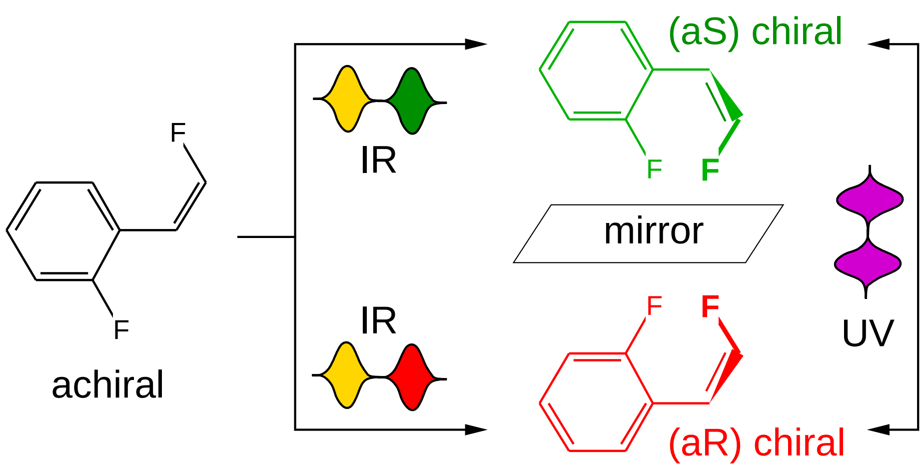


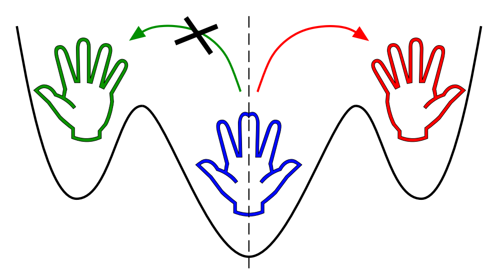

(3*S*,3'*S*)-(*M*,*M*)-*cis*-**2**
>99%

(3*S*,3'*S*)-(*P*,*P*)-*trans*-**2**
>99%

- $> 99\%$ stereoselectivity in both directions
- nanoscale devices: data storage, information processing

## Laser controlled enantioselective isomerization:[2]



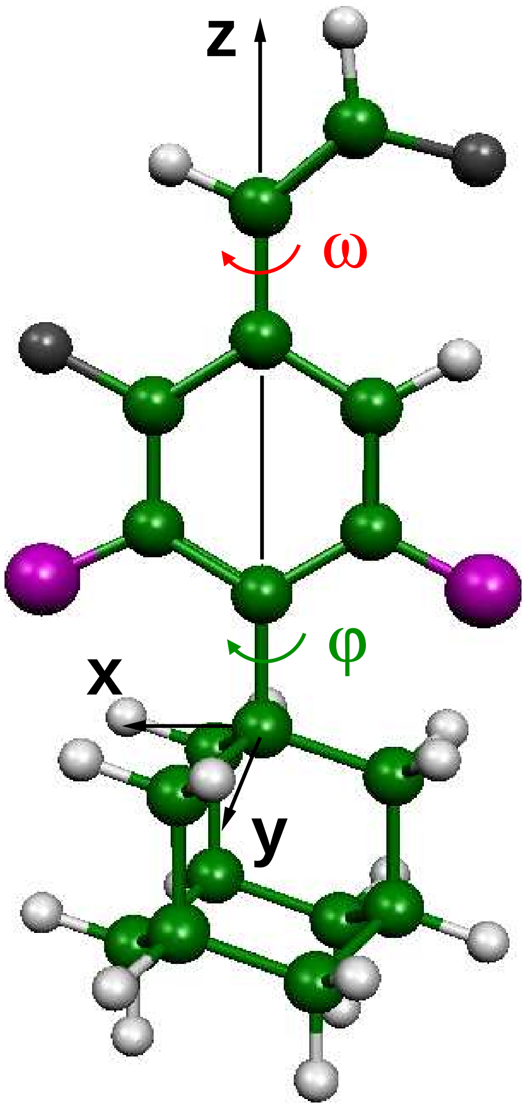



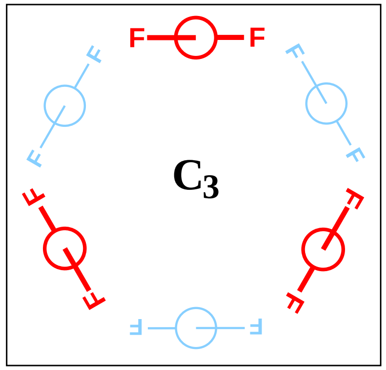
- stereoselective linearly polarized laser pulses
- oriented chiral molecular switch

[1] R. A. van Delden, M. K. J. ter Wiel, B. L. Feringa, *Chem. Comm.*, 200 (2004)
[2] D. Kröner, B. Klaumünzer, *Phys. Chem. Chem. Phys.* **9**, 5009 (2007)

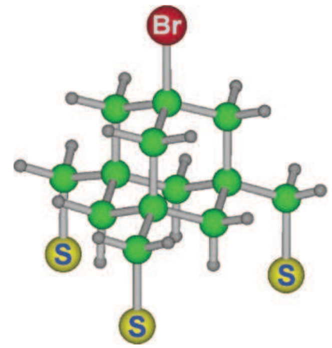
# Surface mounted chiral switch

## Rotational symmetries:[1)]

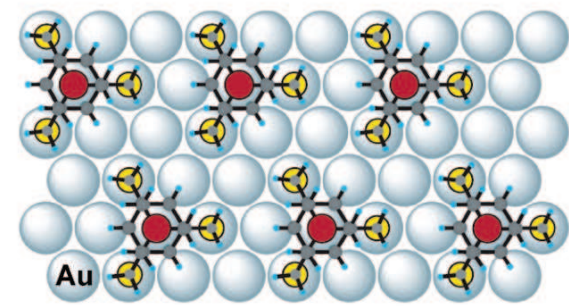


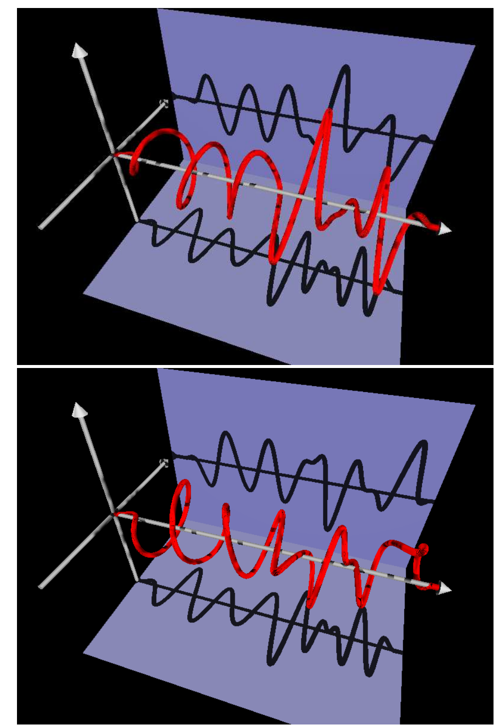

## Rigid molecular tripod:[2)]




Au(111)



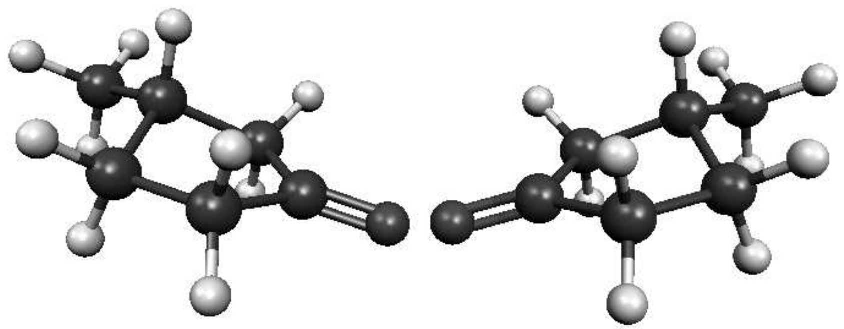

- different orientations
- stochastic pulse optimization[3)]
- stereoselective laser pulse:
  - elliptically polarized
  - equivalent effect for each orientation



[1)] D. Kröner, B. Klaumünzer, T, Klamroth *J. Phys. Chem. A* **112**, 9924 (2008)
[2)] T. Kitagawa, Y. Idomoto, H. Matsubara et al., *J. Org. Chem.* **71**, 1362 (2006)
[3)] T. Klamroth, D. Kröner, *J. Chem. Phys.* **129**, 234701 (2008)

# Chiral recognition

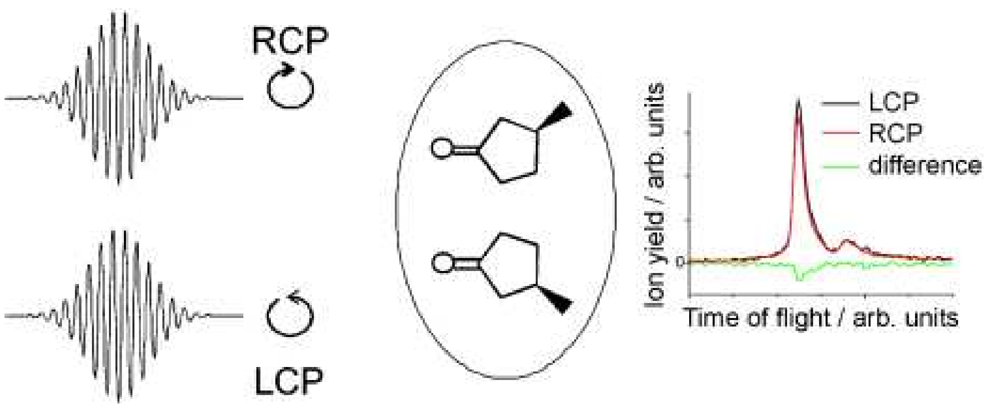
## Enantiospecific electronic excitation:[1)]



(S)−3−Methylcyclopentanon (R)−3−Methylcyclopentanon

- electron wavepacket dynamics
- circularly/elliptically polarized laser pulses
- enantiospecific electronic excitation, for 2 electronic states of chiral molecules[2)]

## Femtosecond-laser mass spectrometry:[3)]

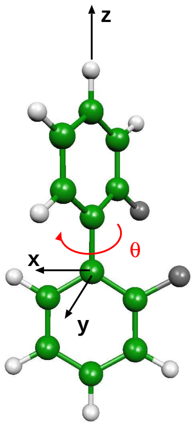



- circular dichroism
- femtosecond laser pulses
- analysis of enantiomers in mass spectrometry[3),4)]

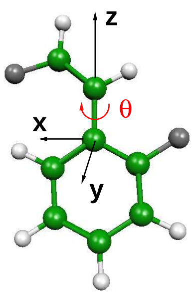
[1)] DFG-Project KR 2942/2
[2)] Y. Ma, A. Salam, *Chem. Phys. Lett.* **431**, 247 (2006)
[3)] H. G. Breuning, G. Urbasch, P. Horsch, J. Codes, U. Koert, K.-M. Weitzel, *Chem. Phys. Chem.* **10**, 1199 (2009)
[4)] U. Boesl, A. Bornschlegl, *Chem. Phys. Chem.* **7**, 2085 (2006)

# Molecular model systems and environment

## Chiral axis:

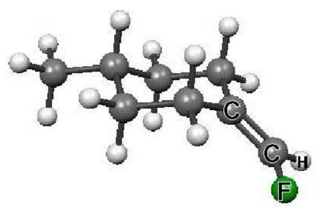



**Biphenyl**

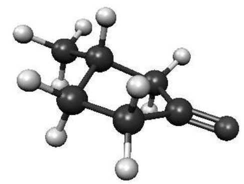



**Styrene**

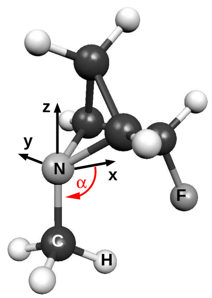
## (Pro)chiral center:




**Cyclohexylidenemethane**[1]



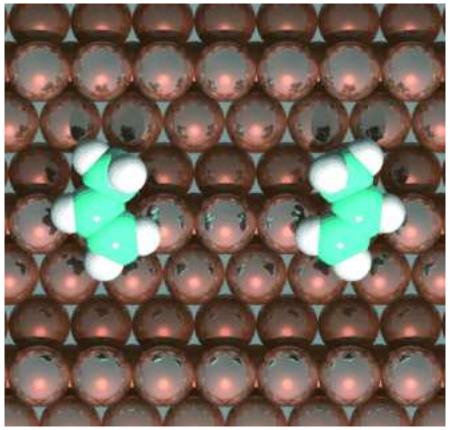
**Cyclopentanone**




**Azabicylcopentane**[2]

- IR/UV stereoselective laser pulse excitation and control
- nuclear and electron quantum dynamics

## Environment: Surface

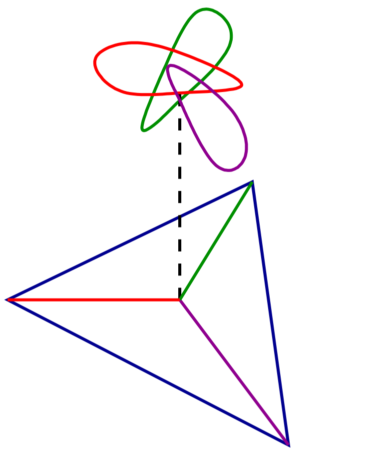


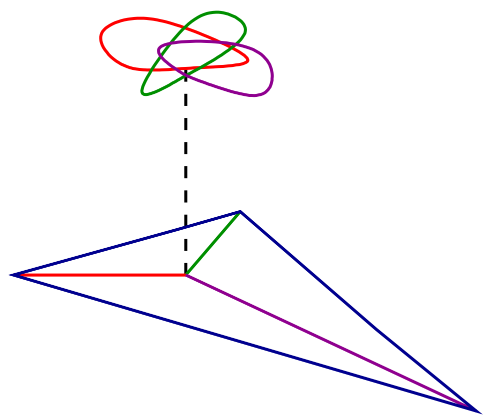
- chiral molecules form domains of unique chirality[3]
- achiral molecules can become chiral when adsorbed: propene@Cu(211) forms chiral adsorbates, STM tip induces conversion into the opposite enantiomer[4]
- enantioselective desorption by laser pulses?
- dissipation, open system quantum dynamics

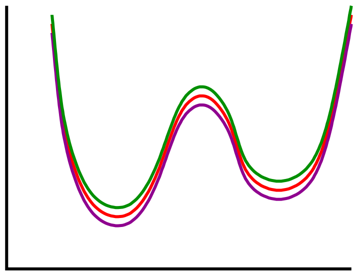
[1] D. Kröner, L. González, *Phys. Chem. Chem. Phys.* **5**, 3933 (2003)
[2] B. Klaumünzer, D. Kröner, *New J. Chem.* **33**, 186 (2009)
[3] M. Ortega Lorenzo, C.J. Baddeley, C. Muryn, R. Raval, *Nature* **404**, 376 (2000)
[4] M. Parschau, D. Passerone, K.-H. Rieder, H. J. Hug, K.-H. Ernst, *Angew. Chem. Int. Ed.* **48**, 4065 (2009)

# Influence of environment or vicinity

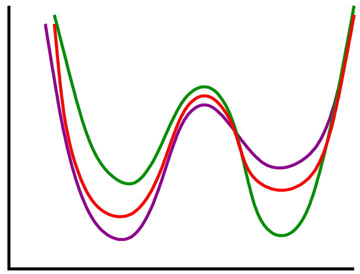
## Symmetric or asymmetric environment:



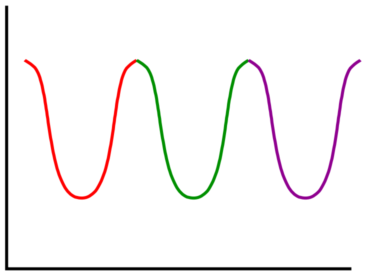




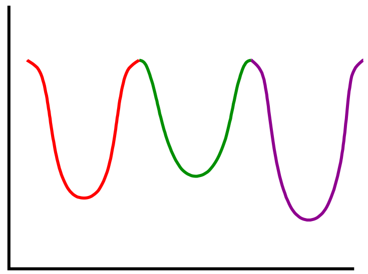
**reaction**



**reaction**

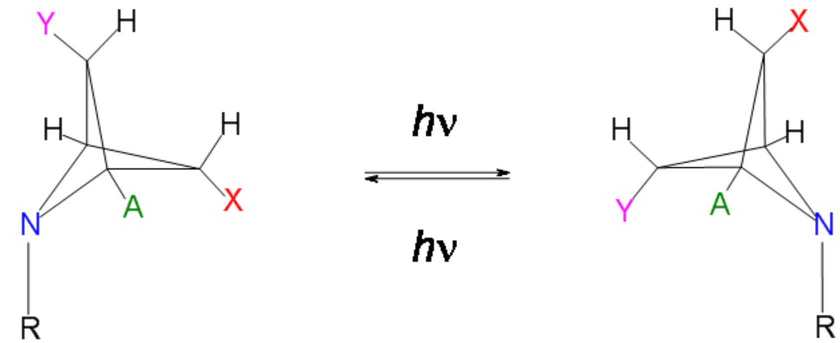


**orientation**



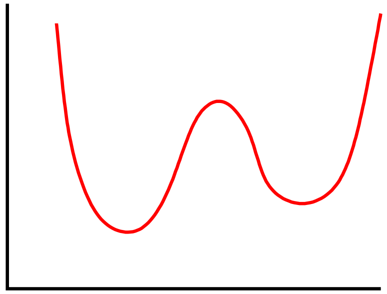
**orientation**

## Symmetric or asymmetric vicitinity:




R : linker/surface

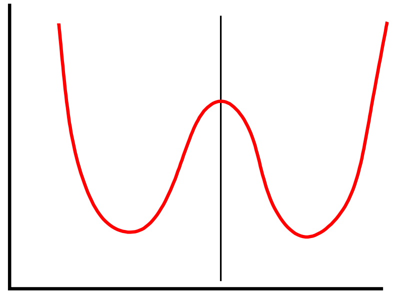
X ≠ Y



**N–inversion**

A ≠ H
⇒ diastereomers

X = Y



**N–inversion**

A = H
⇒ enantiomers