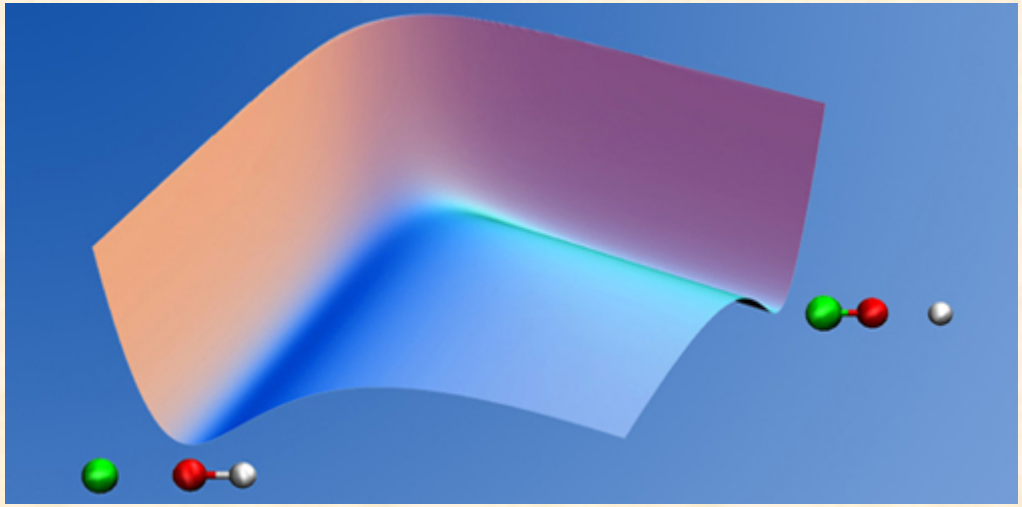
Reaktionsdynamik



V: Mi 13:15 - 14:45
V+Üb: Do 9:45 - 11:15
HS10.119 Seminarraum der PC

Skript: http://www.pci.tu-bs.de/aggericke/PC5
Downloadbereich: http://www.pci.tu-bs.de/aggericke/PC5/download

Reaktionsdynamik

Fundamentales Interesse an der Dynamik chemischer Reaktionen

Beitrag zum Verständnis
komplexer chemischer Reaktionen

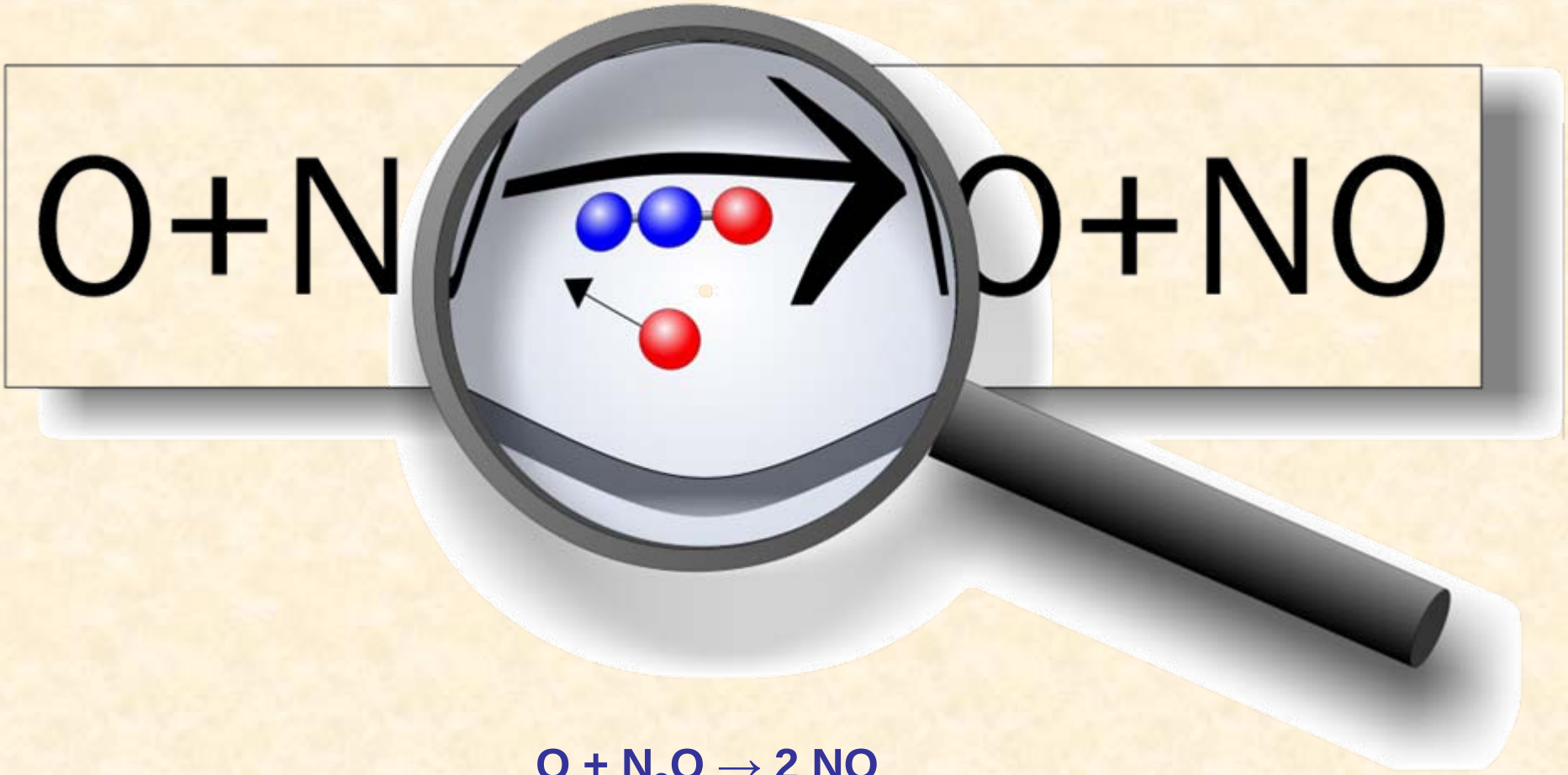
z.B. in der Atmosphärenchemie:

$O_2 + O + M^* \rightarrow O_3 + M$

bisher keine systematischen Studien

Reaktionsdynamik

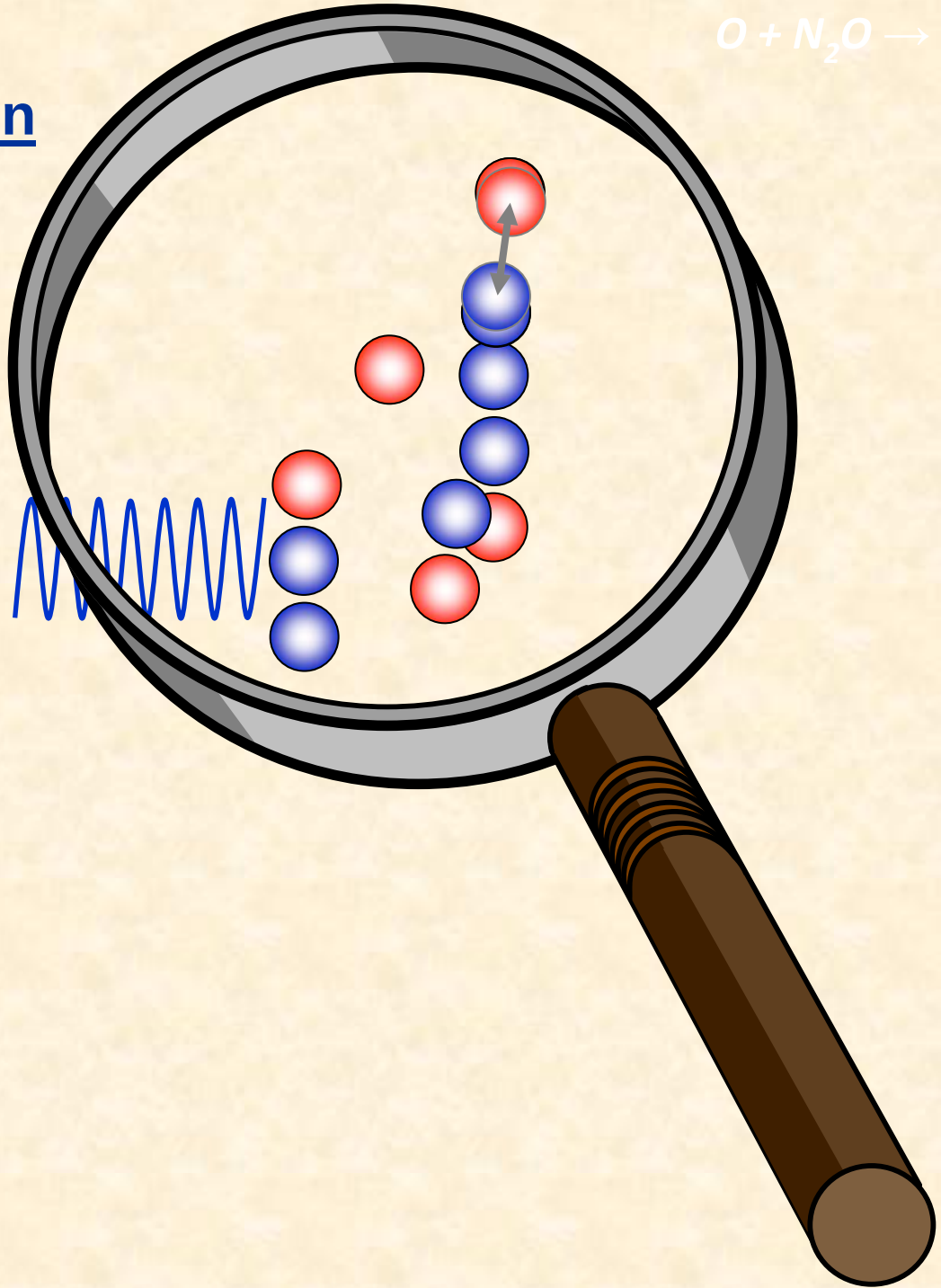
Annäherung durch das Experiment



$O + N_2O \rightarrow 2\ NO$

$O + N_2O \rightarrow 2\ NO$

Reaktionsmechanismen



Unimolekularer Zerfall

Imaging community of the world

Hilfsmittel: Spektroskopie

1) Butler (Chicago, USA)
2) Chandler (Livermore, USA)
3) Continetti (San Diego, USA)
4) Crim (Madison, USA)
5) Houston (Ithaca,USA)
6) Loock (Ontario, Canada)
7) Neumark (Berkeley, USA)
8) Jackson (Davis, USA)
9) North (College Station, USA)
10) Pratt (Argonne, USA)
11) Reisler (Los Angeles, USA)
12) Sanov (Tucson, USA)
13) Suits (Detroit, USA)
14) Wodtke (Santa Barbara, USA)
15) Zare (Stanford, USA)

1) Ashfold (Bristol, UK)
2) Banares (Madrid, Spain)
3) Brouard (Oxford, UK)
4) Drabbels (Lausanne, Switzerl.)
5) Gericke (Braunschweig, Ger.)
6) Janssen (Amsterdam, Netherl.)
7) Kitsopoulos (Heraklion, Greece)
8) Orr-Ewing (Bristol, UK)
9) Parker (Nijmegen, Neth.)
10) Poisson (CNRS Paris, France)
11) Softley (Oxford, UK)
11) Temps (Kiel, Germany)
12) Whitaker (Leeds, UK)

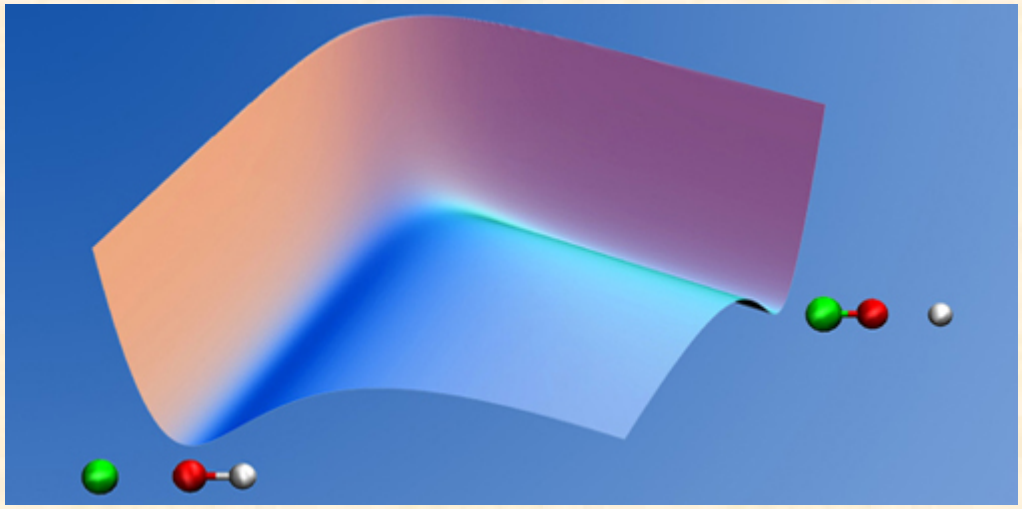
1) Kawasaki (Kyoto, Japan)
2) Kopin Liu (Taipei, Taiwan)
3) Sang Kyu Kim (Daejeon, S. Korea)
4) Suzuki (Wako, Japan)
5) Yang (Dalian, China)
6) Zhang (Wuhan, China)

Reaktionsdynamik

Annäherung durch theoretische Beschreibung

- Kinetik
- Übergangszustand
- Statistische Thermodynamik
- Quantenmechanik

Reaktionsdynamik



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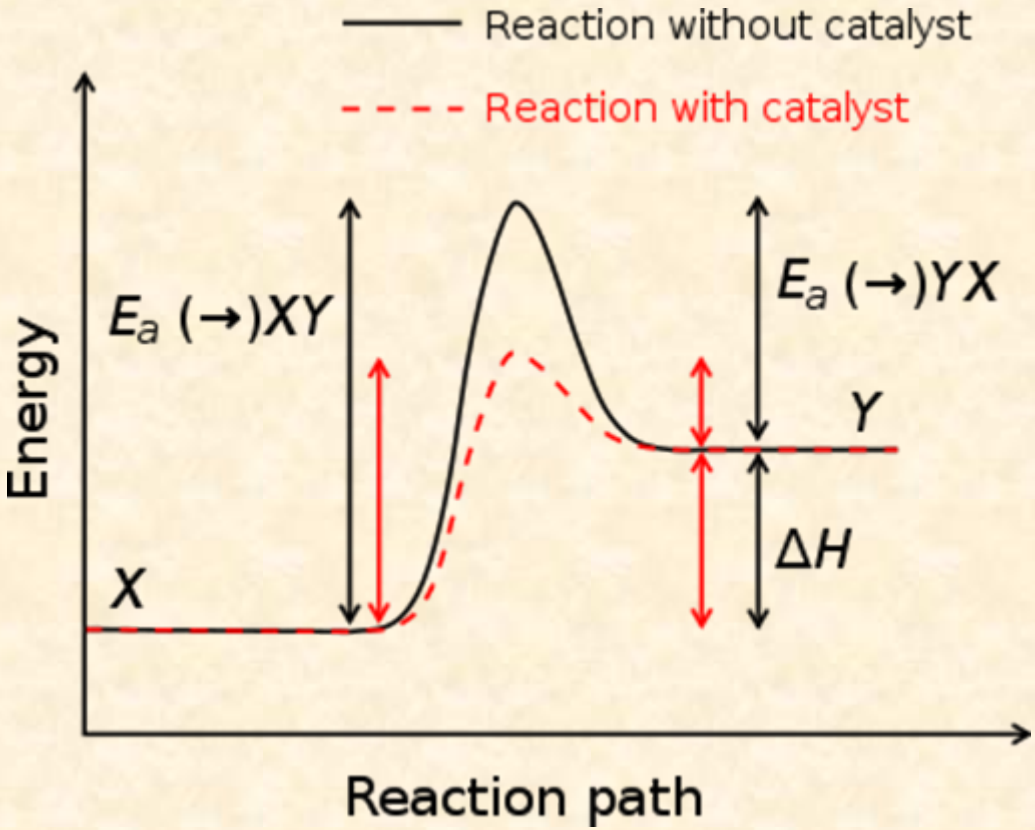
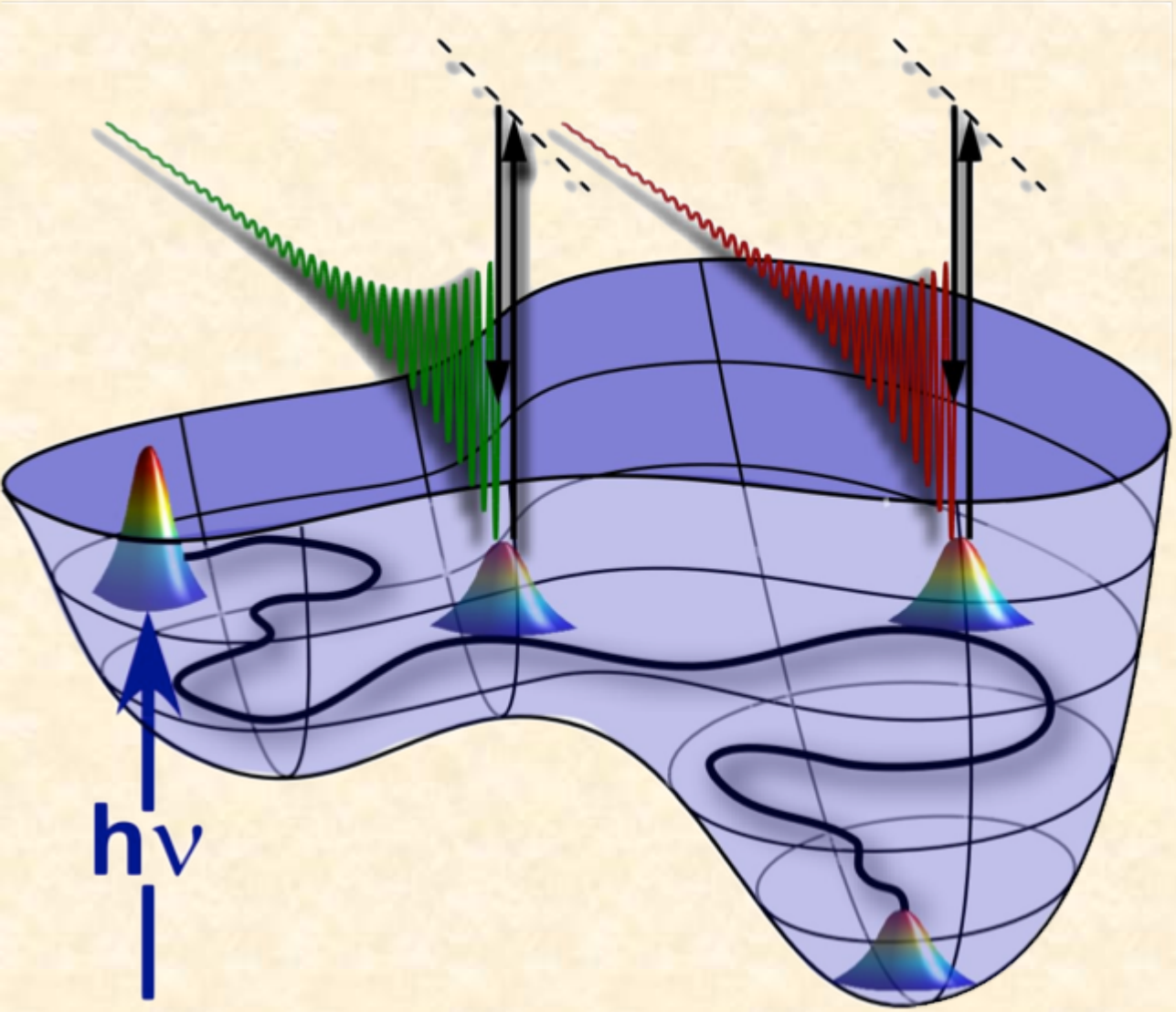
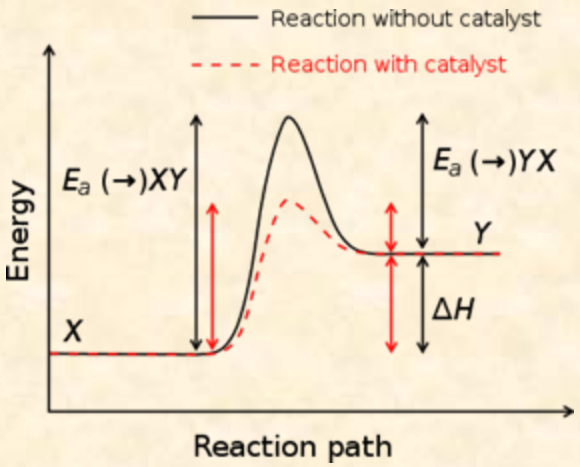
Reaktionsdynamik

Die naive Sichtweise

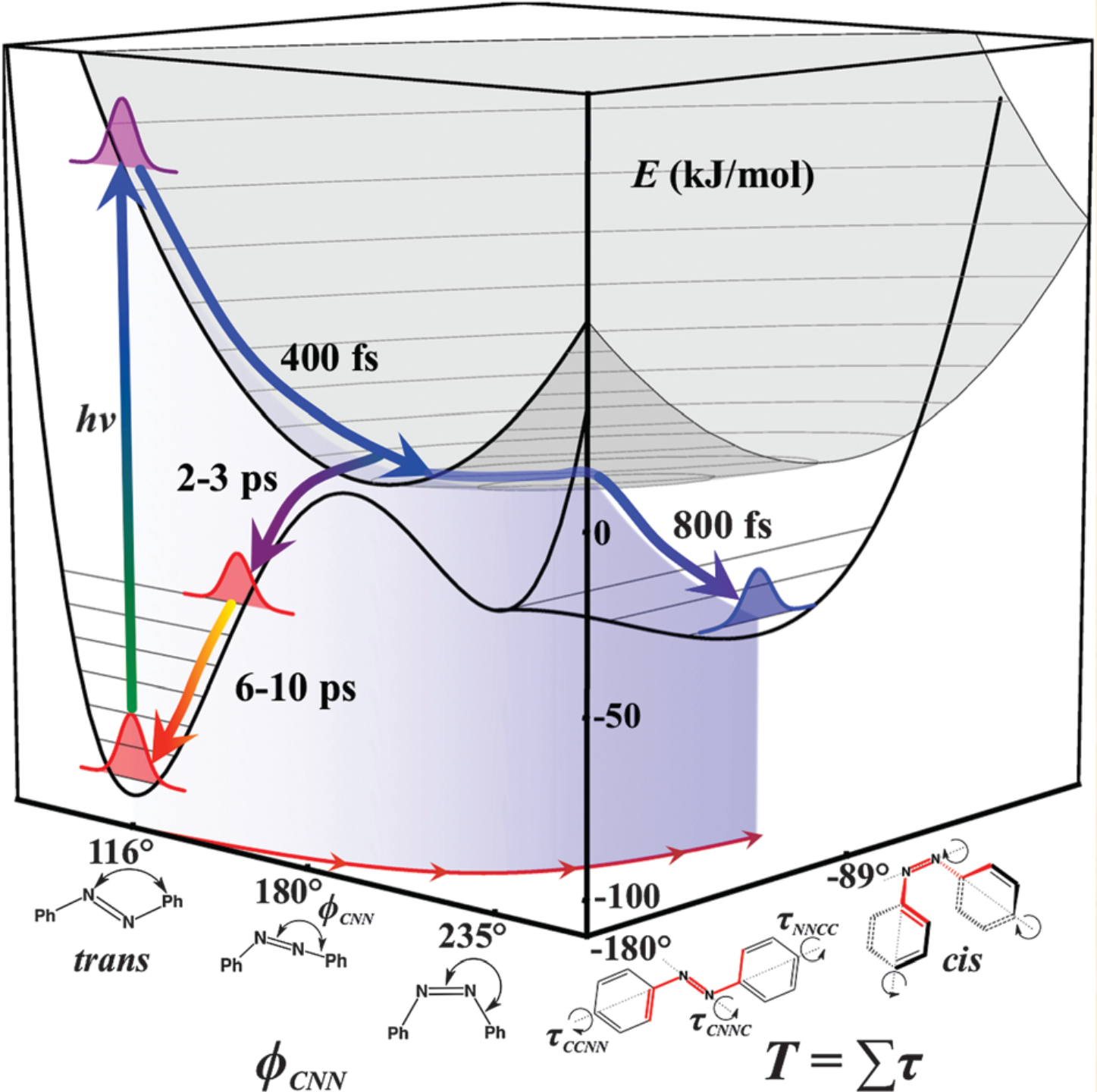


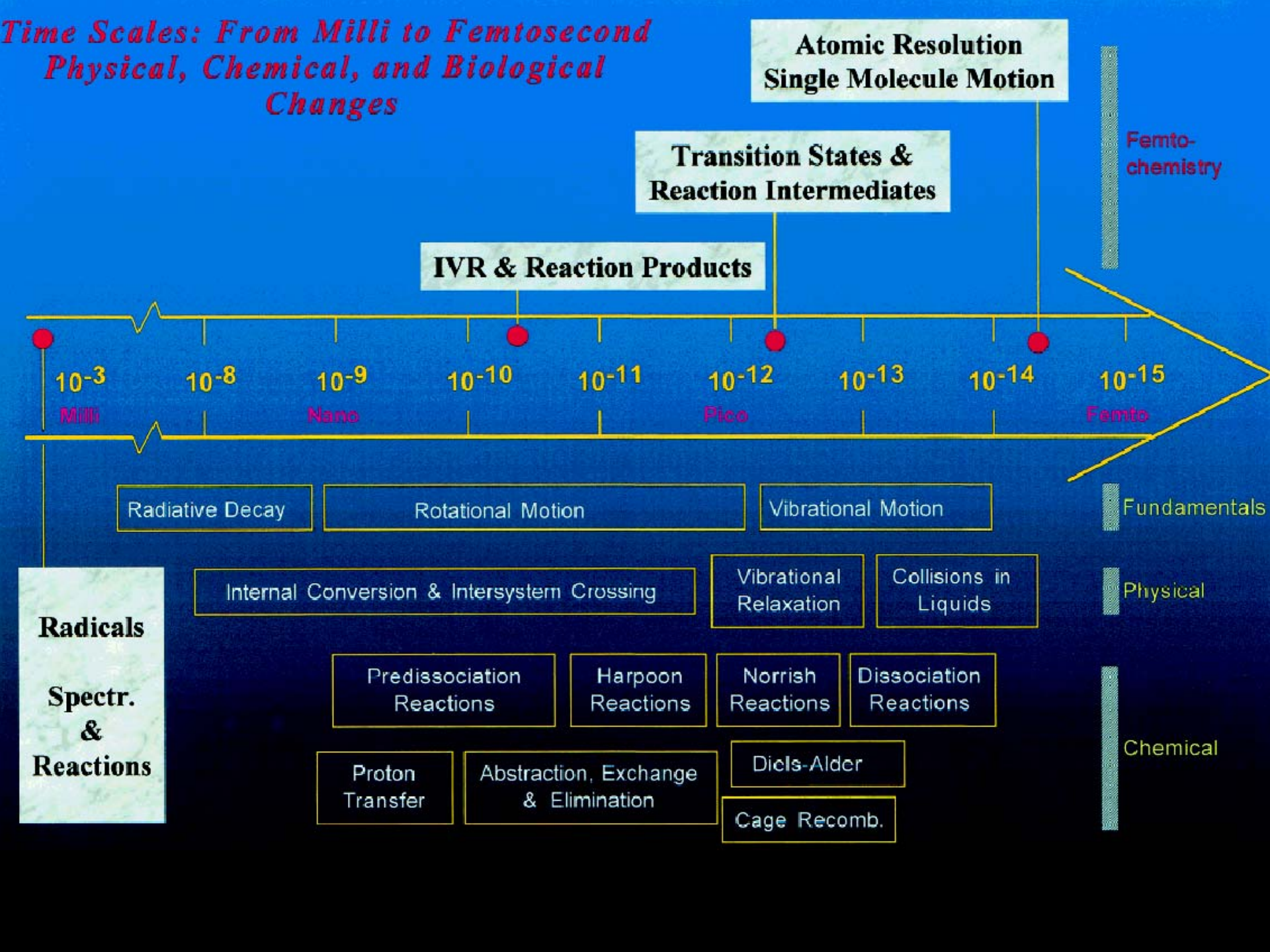
Der verschlungene Reaktionsweg



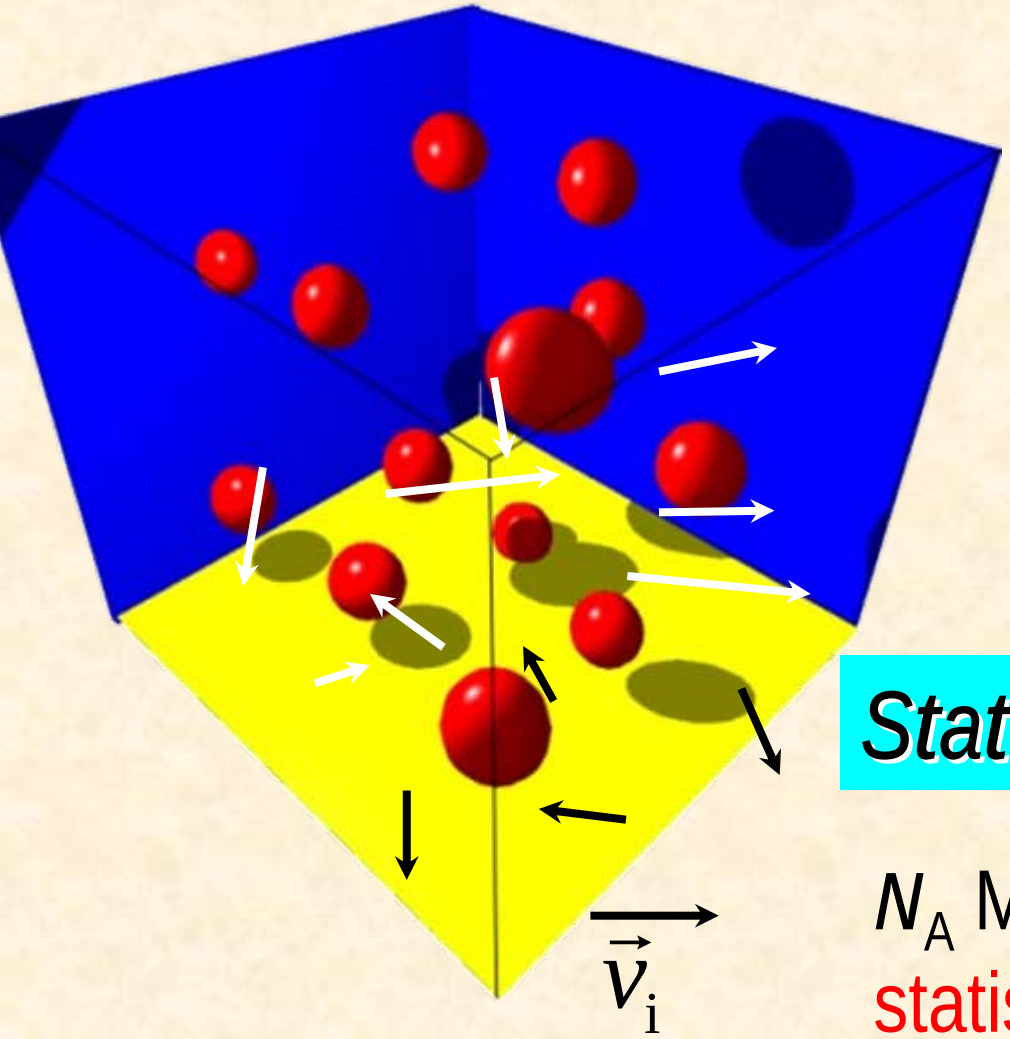


Azobenzene Dynamics in PCCP




Time Scales: From Milli to Femtosecond
Physical, Chemical, and Biological
Changes
Atomic Resolution
Single Molecule Motion
Transition States &
Reaction Intermediates
IVR & Reaction Products
Femto-
chemistry
10-3
Milli
10-8
10-9
Nano
10-10
10-11
10-12
Pico
10-13
10-14
10-15
Femto
Radiative Decay
Rotational Motion
Vibrational Motion
Fundamentals
Radicals
Spectr.
&
Reactions
Internal Conversion & Intersystem Crossing
Vibrational
Relaxation
Collisions in
Liquids
Physical
Predissociation
Reactions
Harpoon
Reactions
Norrish
Reactions
Dissociation
Reactions
Chemical
Proton
Transfer
Abstraction, Exchange
& Elimination
Diels-Alder
Cage Recomb.

Das Problem



$$m_i \ddot{\vec{r}}_i = -\vec{\nabla} V(\vec{r}_1, \vec{r}_2, \cdots, \vec{r}_N)$$

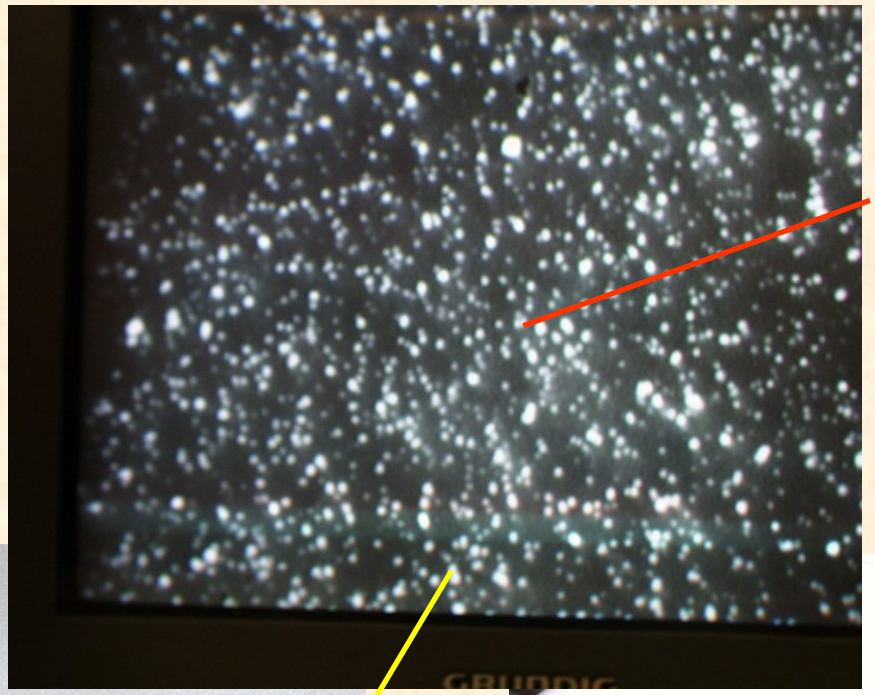
$$i = 1, ..., N$$

$$N \approx N_A = 6.022 \cdot 10^{23}$$

Statistische Beschreibung!!

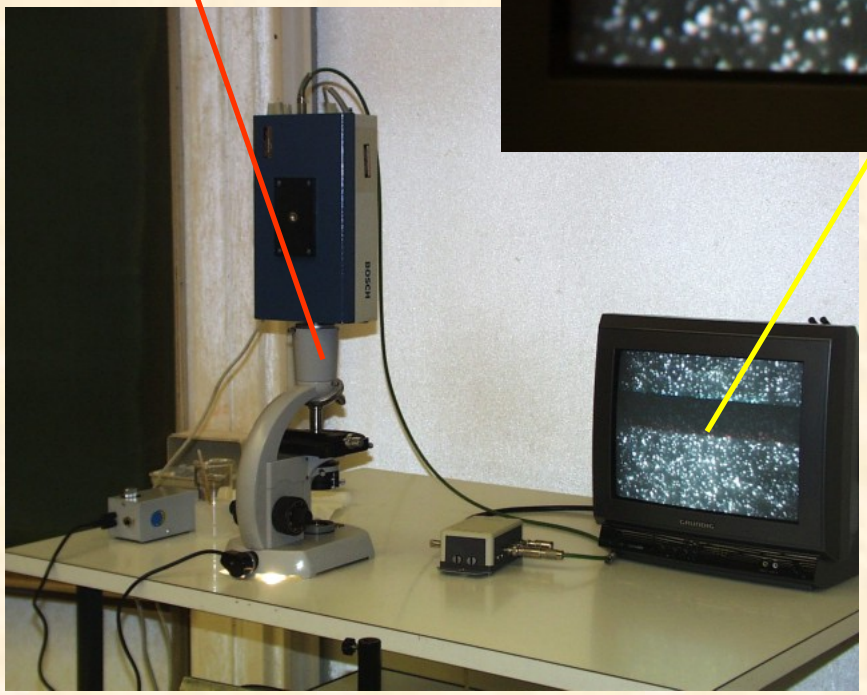
N_A Moleküle führen statistisch unabhängige Bewegungen aus.

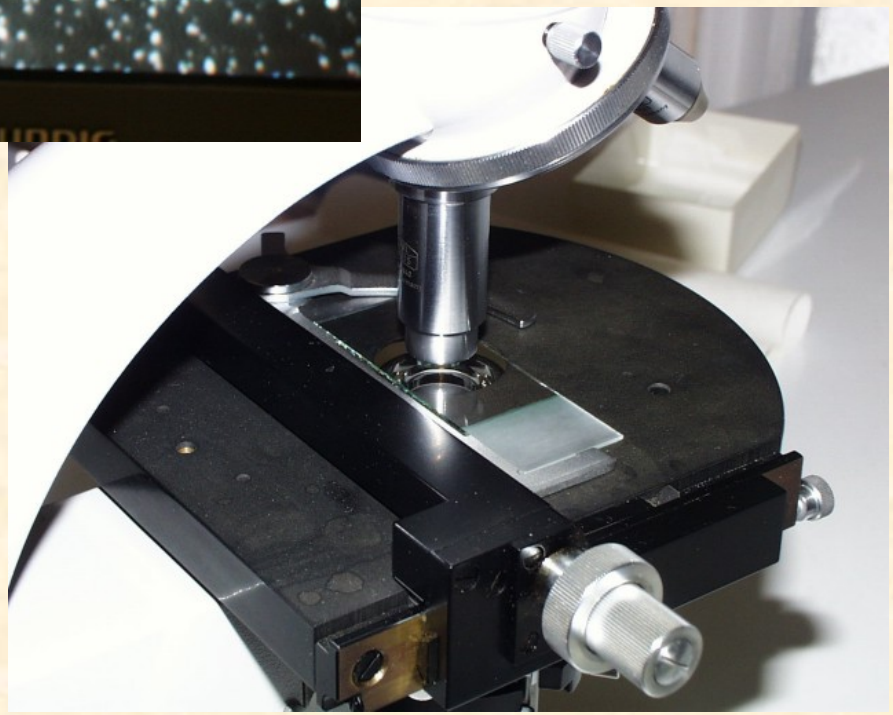
Brown‘sche Molekular-bewegung



Die in einer Lösung schwimmenden TiO_2 Partikel führen Zitterbewegungen aus

Mikroskop (x400)

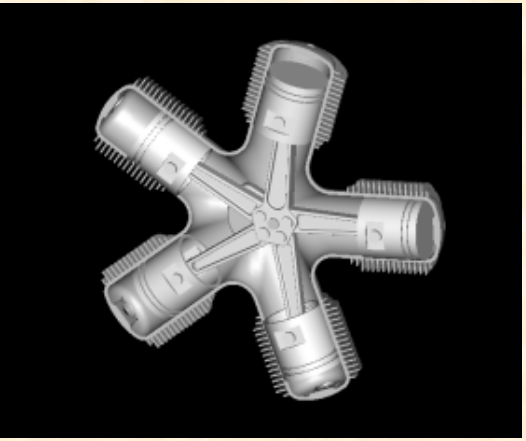




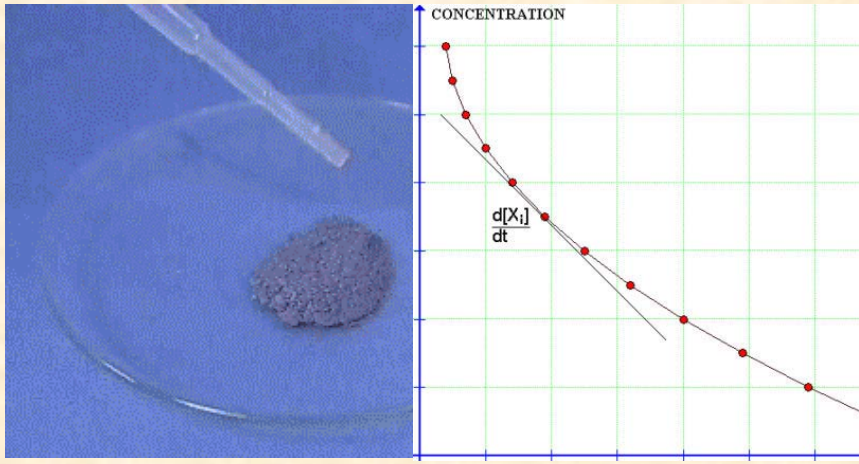
Einzelne Moleküle

Grundlagen der Reaktionsdynamik

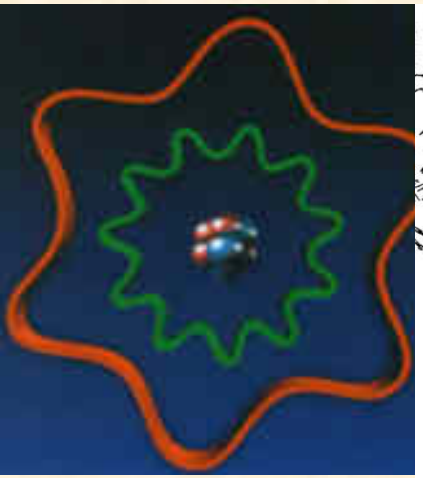
Thermodynamik



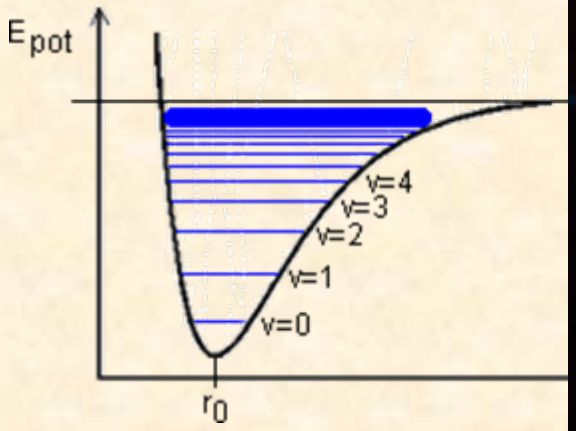
Chemische Kinetik



Quantenmechanik



Spektroskopie



Themen für kommendes Seminar/Übung

- Hauptsätze der Thermodynamik
- Fundamentalgleichungen der Thermodynamik
- Reaktionsordnungen
- Zusammengesetzte Reaktionen
- Gleichgewichtsreaktionen $A \underset{\leftarrow}{\rightarrow} B \rightarrow C$
- Energien in der Quantenmechanik: Rotation, Vibration, Feinstruktur (Spin-Bahn)

Literatur

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- P.W. Atkins, "Physikalische Chemie" ISBN-10: 3527315462 , Wiley / VCH, 2006
- H.Kuhn, H.-D. Försterling, "Principles of Physical Chemistry", John Wiley, 2009, ISBN-13: 978-0470089644
- R.D. Levine, R.B. Bernstein "Molekulare Reaktionsdynamik" Teubner, 1991, ISBN: 3-519-03507-3
- Gerd Wedler und Hans-Joachim Freund , "Lehrbuch der Physikalischen Chemie" 6. Auflage, VCH, 2012, ISBN-13: 978-3527329090
- Sehr gute Skripte im Internet