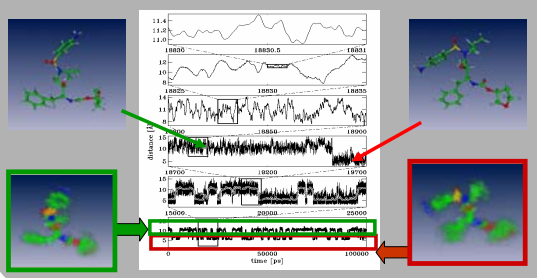
UP I: Konformationsdynamik von Polypeptiden

Kooperationen: TP B7 / C2

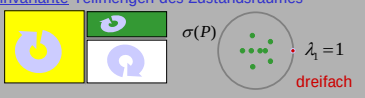
Algorithmen zur Konformations-Dynamik

Konformationen und Metastabilität

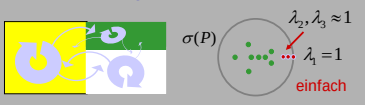


Transfer-Operatoren

- invariante Teilmengen des Zustandsraumes

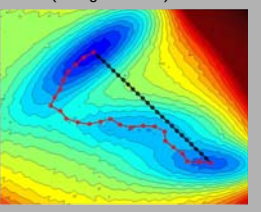


- metastabile Teilmengen des Zustandsraumes



⇒ Identifizierung durch spektrale Struktur

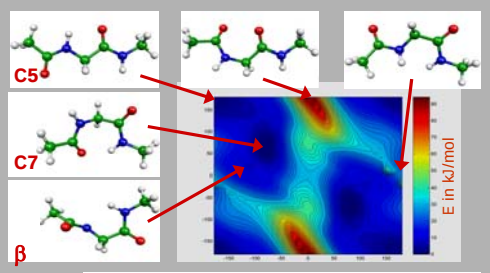
Übergangspfade
(String-Methode)

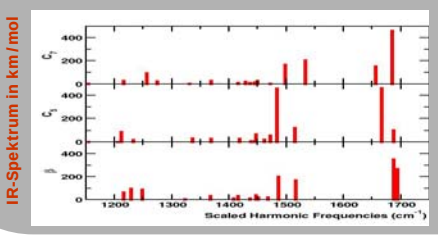


⇒ Verbindung zur **Quanten-Klassik**

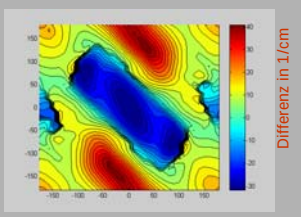
Zeitabhängige Schwingungs-Spektroskopie (Beispiel: Glyzin-Dipeptid)

Potentialfläche B3LYP/ 6-31 +G(d) und Konformationen

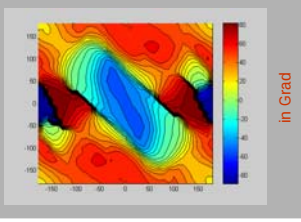




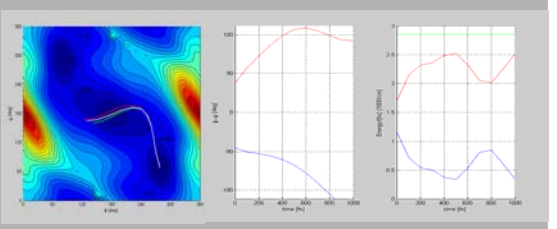
Adiabatische Amid-I Frequenzen



Diabatischer Mischungswinkel

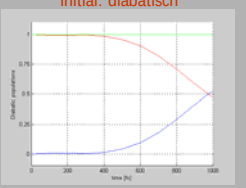


Wellenpaketdynamik ($C_7 \rightarrow C_5$)

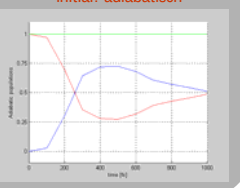


Populationsdynamik

initial: diabatisch

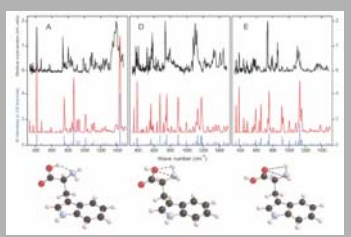


initial: adiabatisch



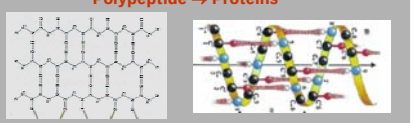
Systeme

Aromatische Aminosäuren (Beispiel: Tryptophan)

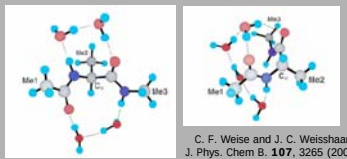


G. Meijer, G. v. Helden, et al. Phys. Rev. Lett. **91**, 203003 (2003)

Polypeptide → Proteins



Mikrosolvatation (Beispiel: Alanain-Dipeptide)



C. F. Weise and J. C. Weisshaar J. Phys. Chem B. **107**, 3265 (2003)

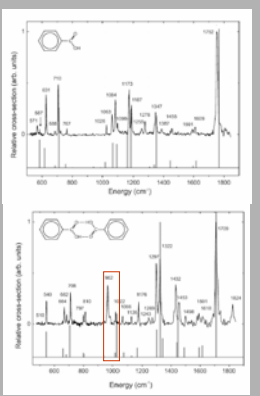
Methoden

Potentielle Energie

- Kraftfelder vs. „ab initio“
- Hartree-Fock vs. DFT

Schwingungsspektren

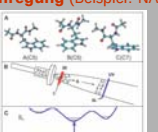
- Volle Hesse-Matrix vs. Unterraum (AKIRA)
- Harmonisch vs. Anharmonisch (Beispiel: Benzoe-Säure)



G. Meijer, G. v. Helden, et al. J. Chem. Phys. **119**, 11180 (2003)

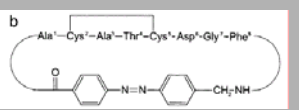
Steuerung ?!?

IR-Anregung (Beispiel: NATMA)



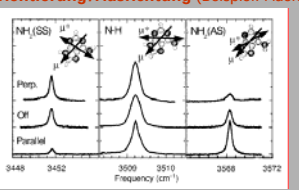
B. C. Dian, A. Longarte, T. S. Zwier Science **296**, 2396 (2002)

Lichtinduzierte Isomerisierung (Beispiel: Zyklopeptid)



Hamm, Wachtveitl, Zinth PNASS **100**, 6452 (2003)

Orientierung / Ausrichtung (Beispiel: Adenin)



F. Dong, R. Miller Science **298**, 1227 (2002)