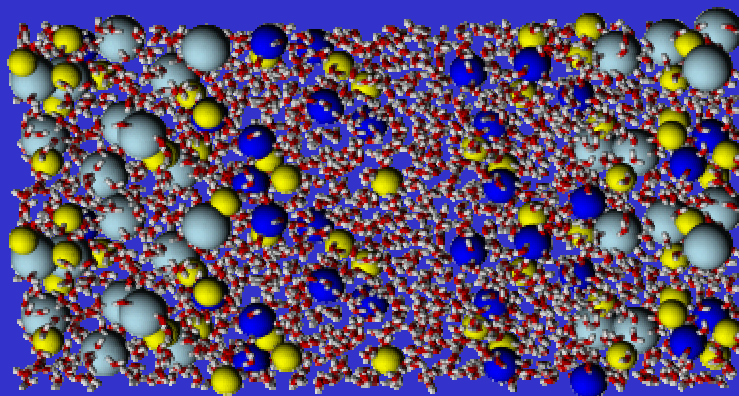




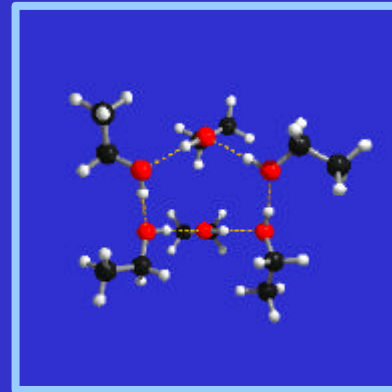
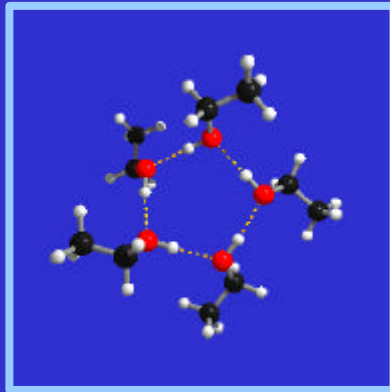
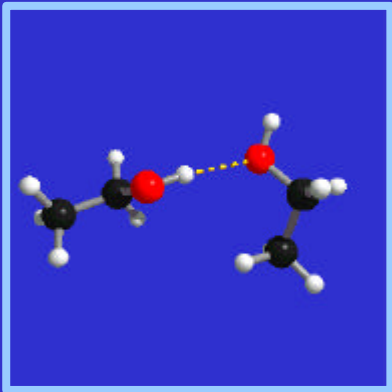
Modellierung und Simulation in der Chemie

Vom Molekülcluster zum Protein und darüber hinaus

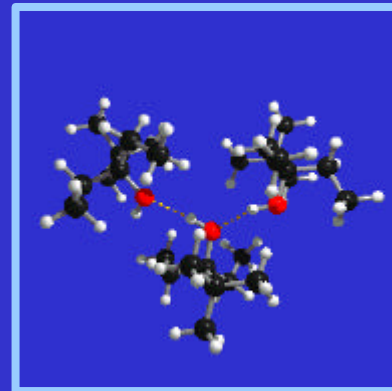
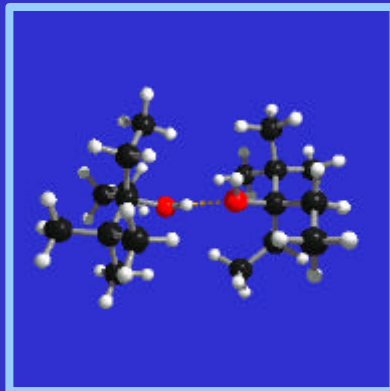
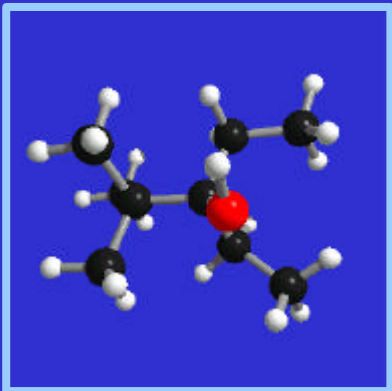


Arbeitsgruppe Prof. Alfons Geiger
Physikalische Chemie, Universität Dortmund

Ab initio Berechnung H-brücken-gebundener molekularer Cluster

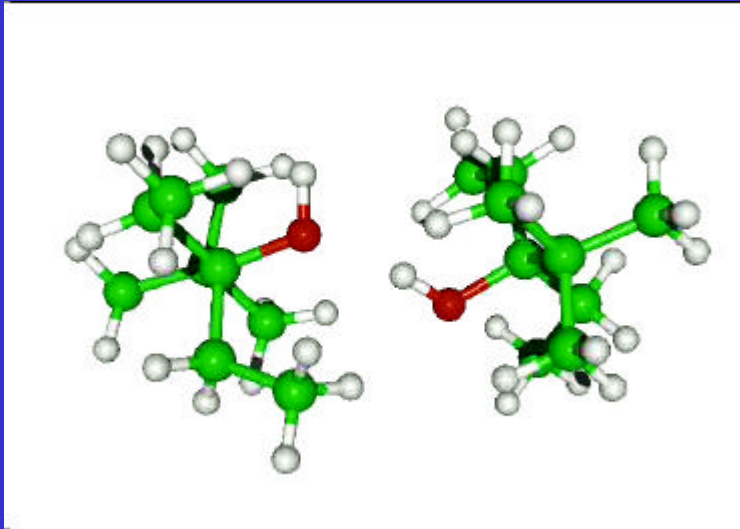


ethanol



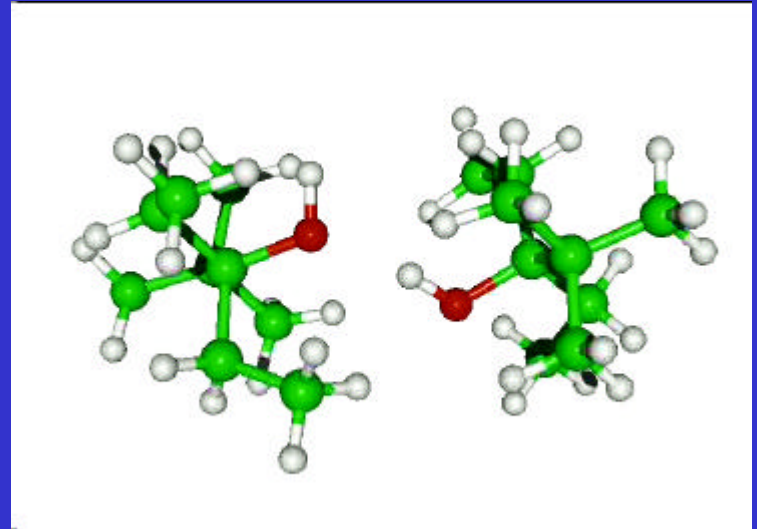
2,2-dimethyl-3-ethyl-3-pentanol (dmep)

Intermolekulare Schwingungen



Streckschwingung der H-Brücke

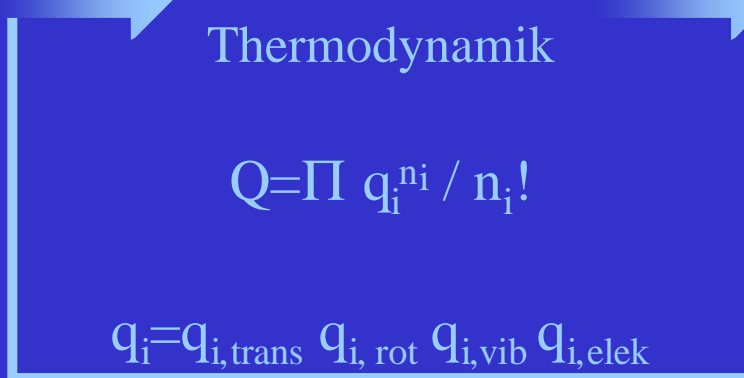
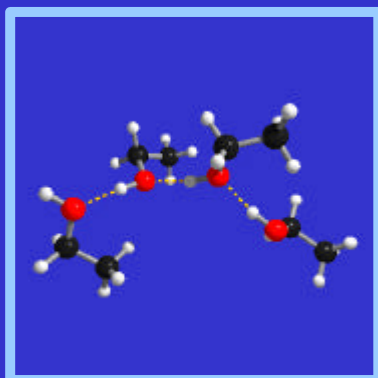
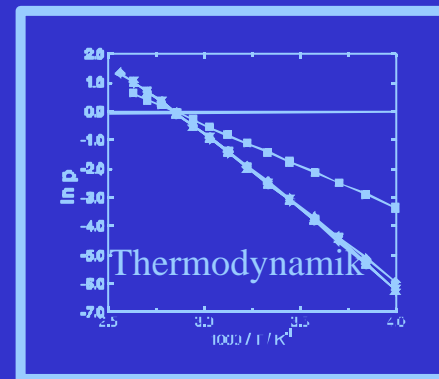
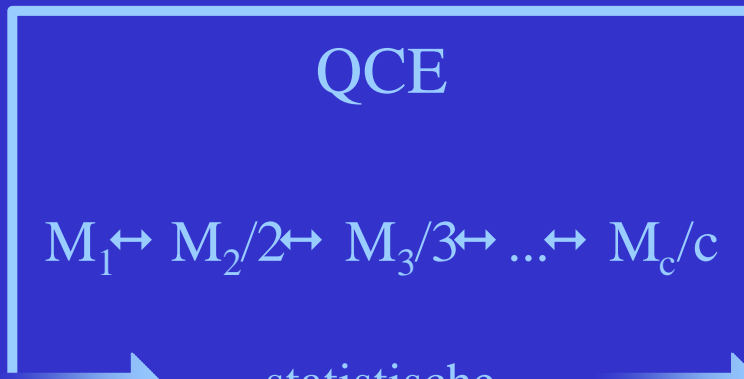
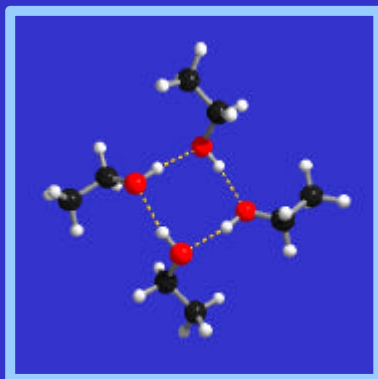
(88 cm^{-1})



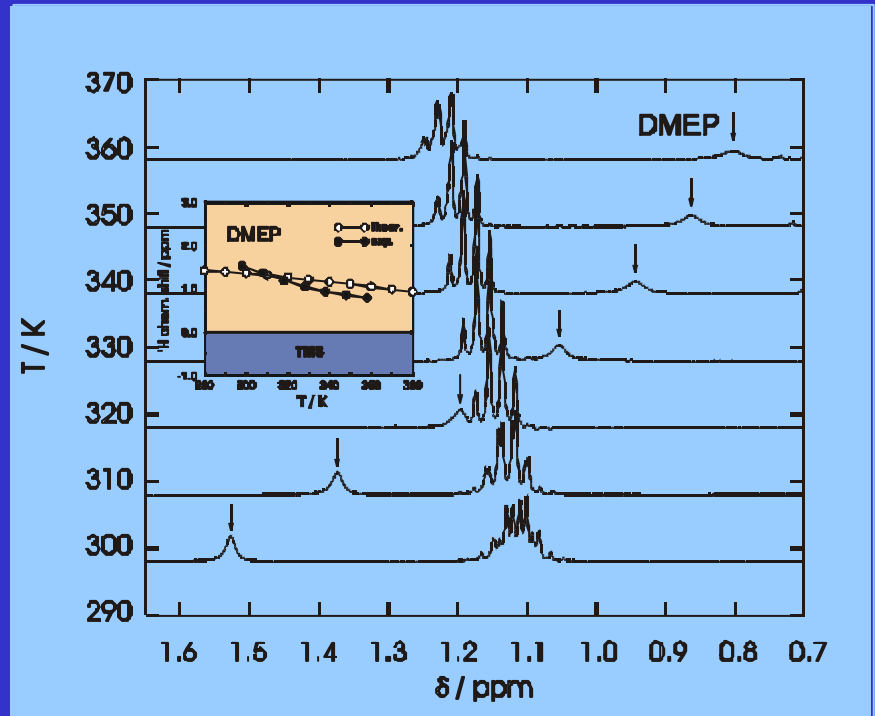
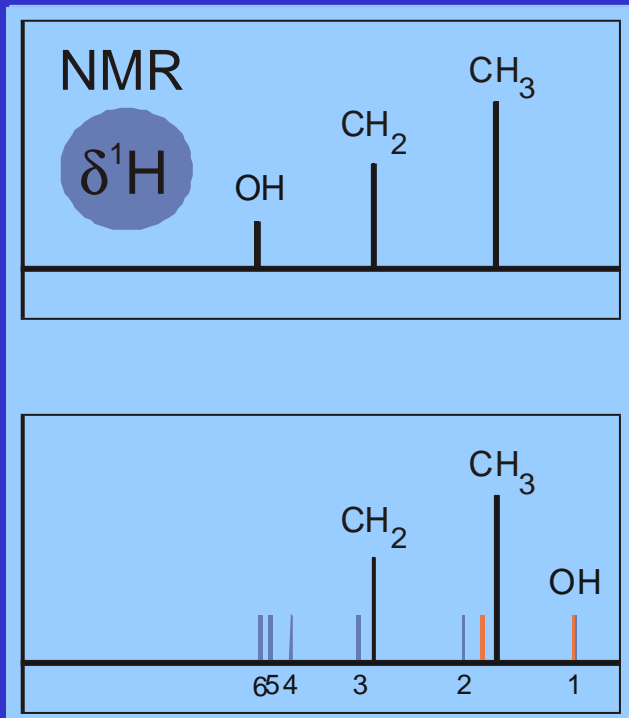
Deformationsschwingung der H-Brücke

(110 cm^{-1})

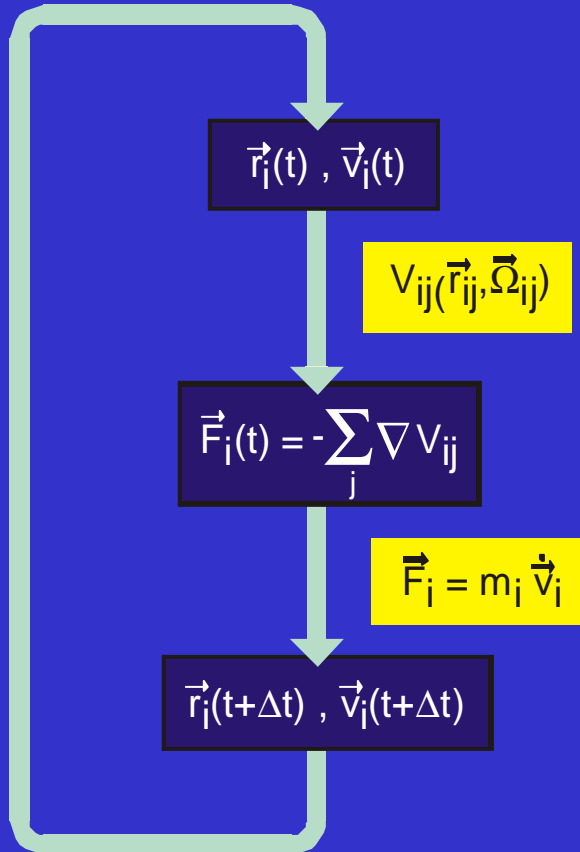
Quantum Cluster Equilibrium (QCE) Modell



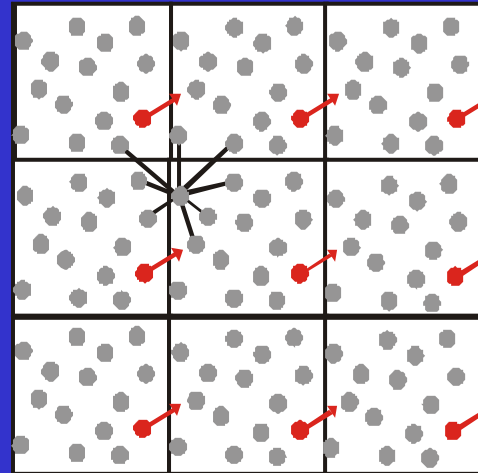
NMR chemische Verschiebungen



Molekulardynamik Simulation



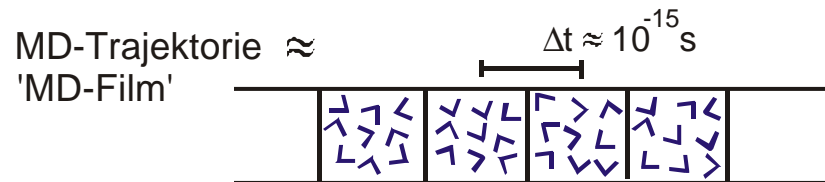
Iteratives Lösen
der Newton'schen
Bewegungsgleichung



$$\rho = N / V$$

Flüssigkeiten
sind wechselwirkende
Vielteilchen-Systeme.

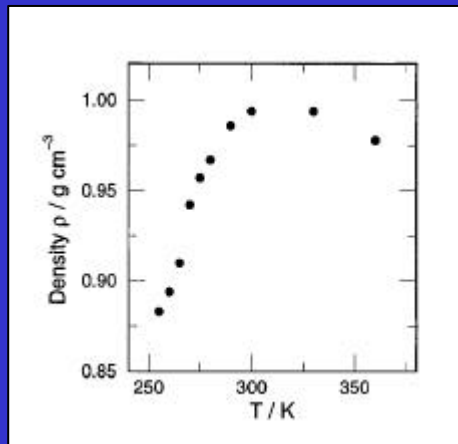
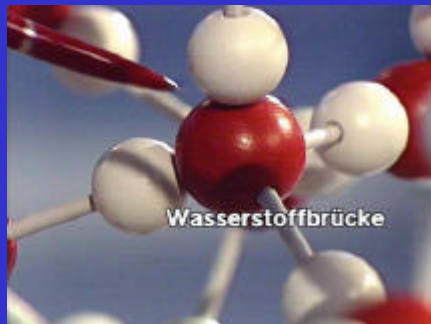
Verwendung
periodischer
Randbedingungen in
der Simulation.



Messgrößen
sind Ensemble-
mittelwerte

$$\langle F(\vec{r}^N(t), \vec{v}^N(t)) \rangle$$

Metastabiles unterkühltes Wasser



**Molekulardynamische
Simulation**

des ST2-Wassers

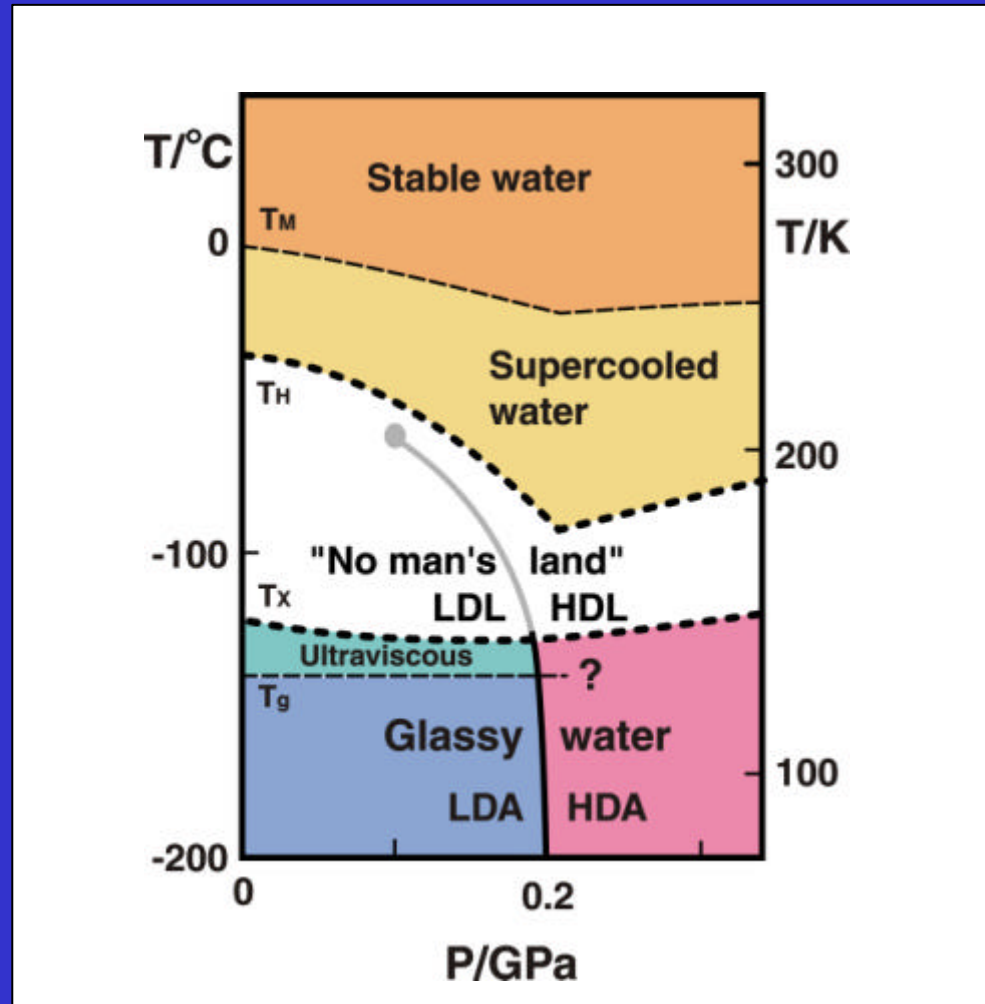
bei

330 K

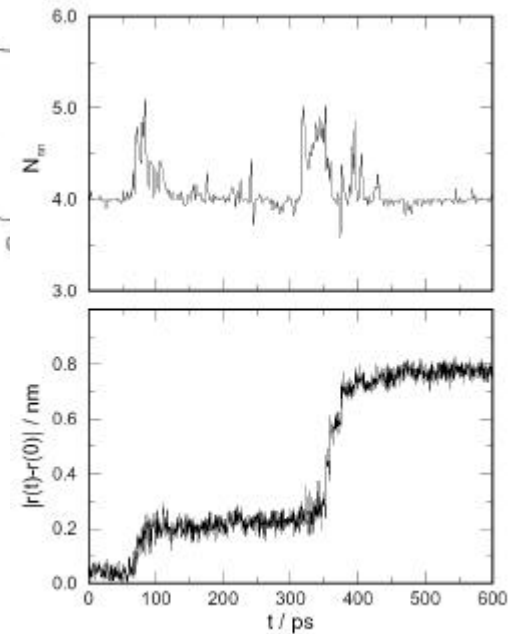
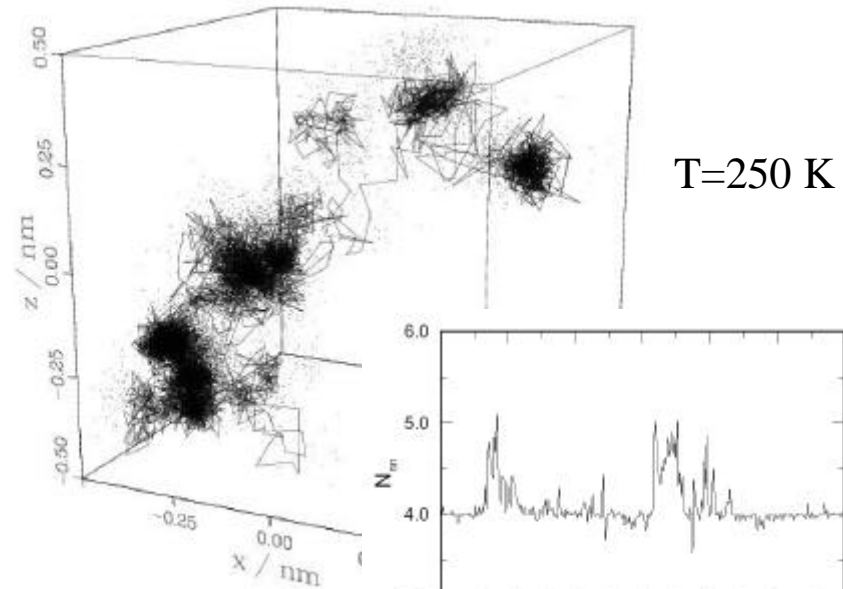
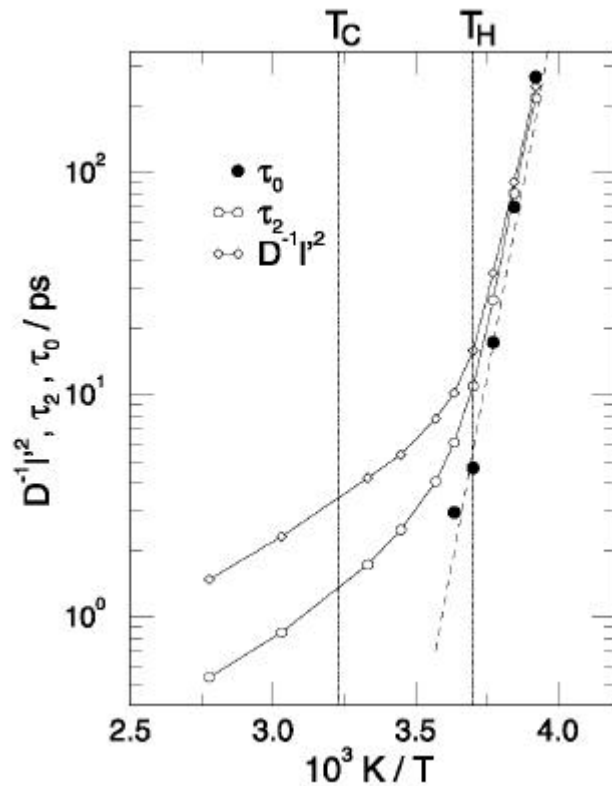
330 K, 270 K, 250 K

- **Dunkel: Stark verzerrte Tetraeder**
- **Hell: Nahezu ideale Tetraeder**

Existenzbereich des flüssigen Wassers: Waters no man's land



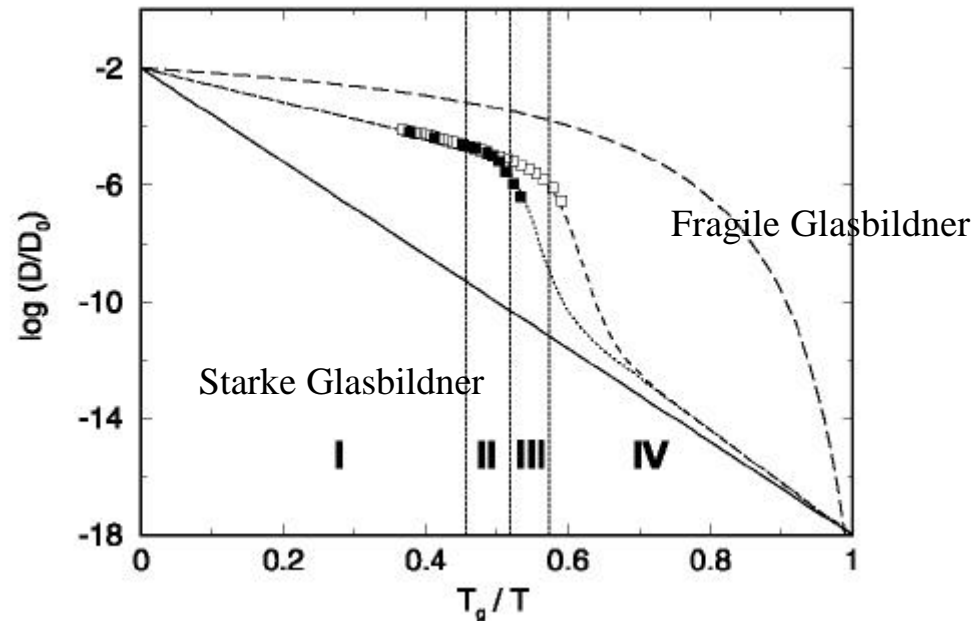
Sprungdiffusion im unterkühlten Wasser



Veränderung des Diffusionsmechanismus im unterkühlten Wasser

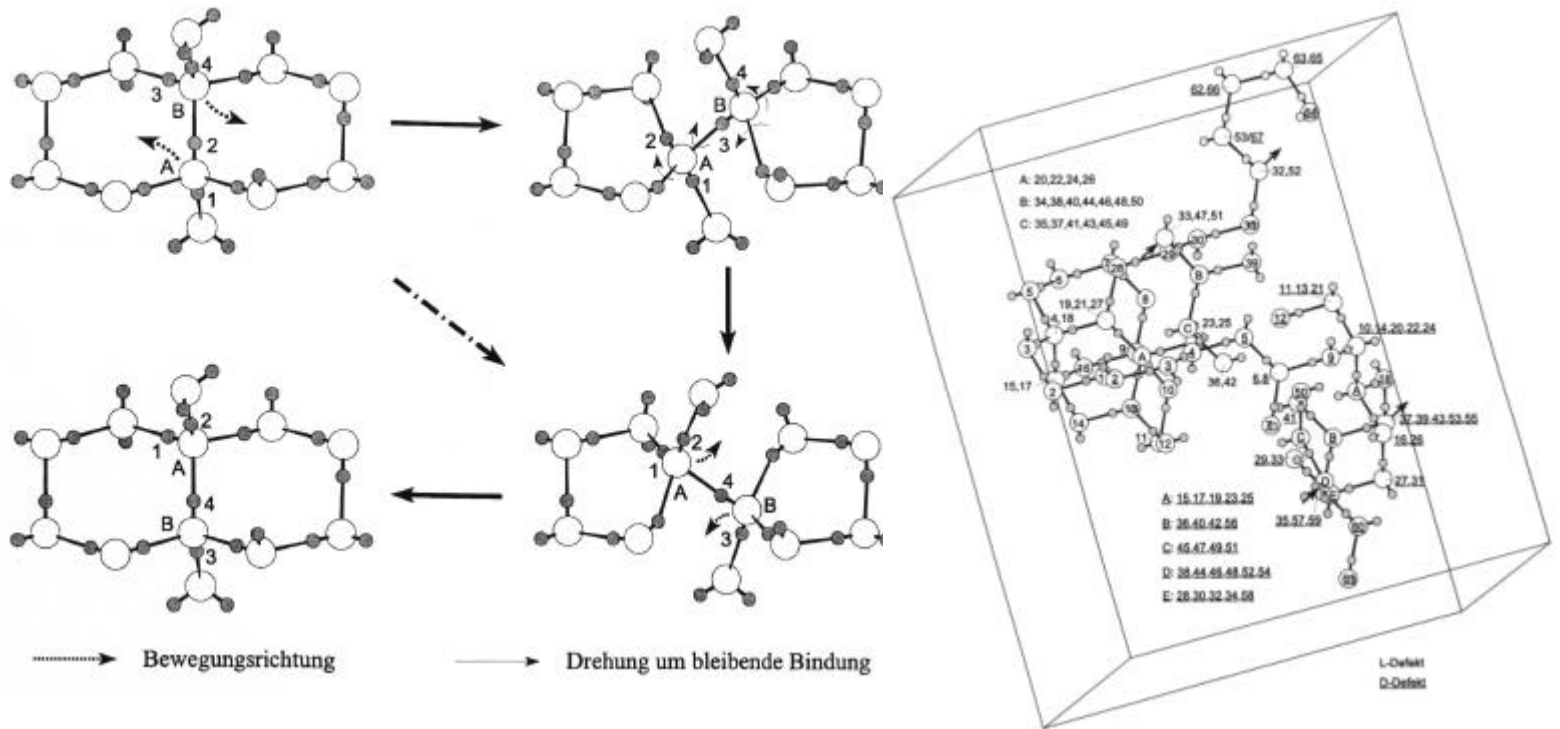
Dynamik unterkühlter Flüssigkeiten: Spezialfall „tetrahedral liquids“

„Angell“-Plot des Diffusionskoeffizienten



Tetraedrische Flüssigkeiten nehmen eine Zwischenposition ein

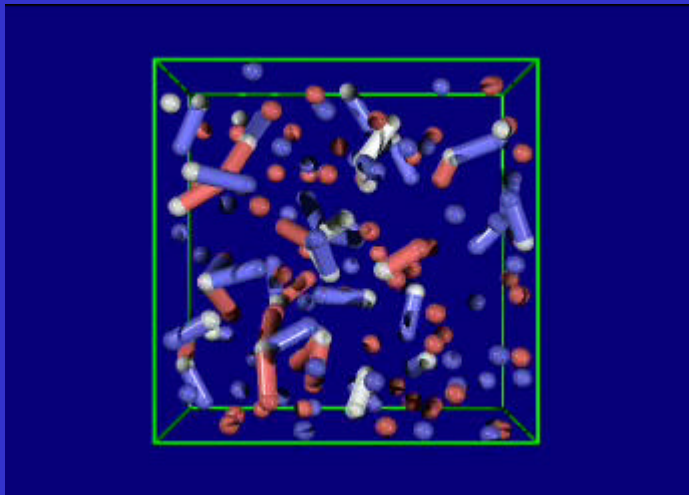
Defektdynamik im überhitzten Eis



Analogie zur Defektdynamik im Eis (hier Simulation) liefert eine mögliche Erklärung für die molekulare Dynamik in der superviskosen Flüssigkeit (Bereich: IV)

Wäßrige Elektrolytlösungen

Bevorzugte Assoziation von hydrophoben Teilchen und Anionen (Hofmeister-Serie)



Wäßrige Lösungen:

$c(X^+Y^-) = 1.6 \text{ mol/l}$

$c(\text{Xe})=0.8 \text{ mol/l}$

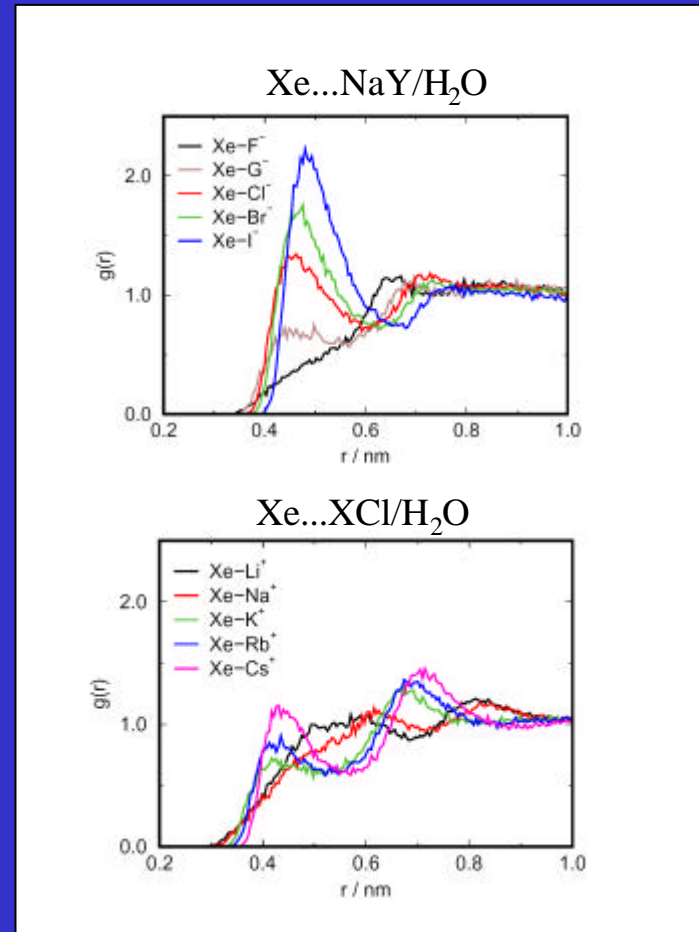
$T=300 \text{ K}$, $p=1 \text{ atm}$

Film (oben):

Blau: Chlorid

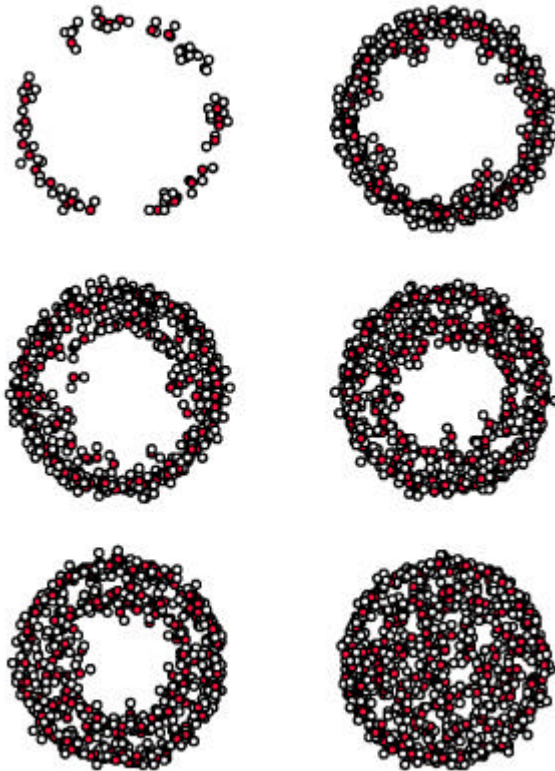
Rot: Natrium

Weiß: Xenon

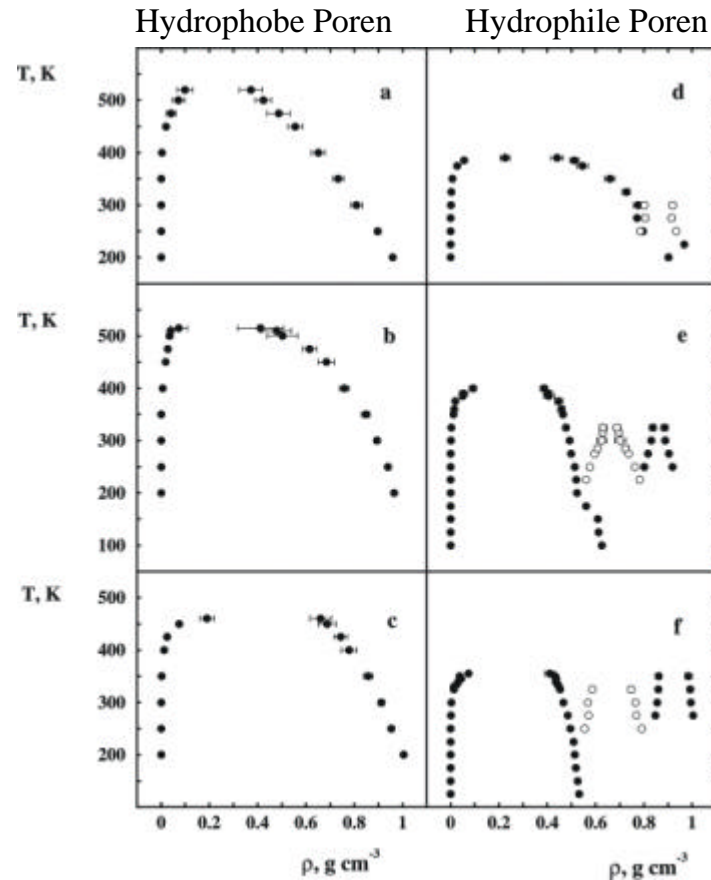


Phasengleichgewichte: Wasser in Poren

Wasser in hydrophiler Pore

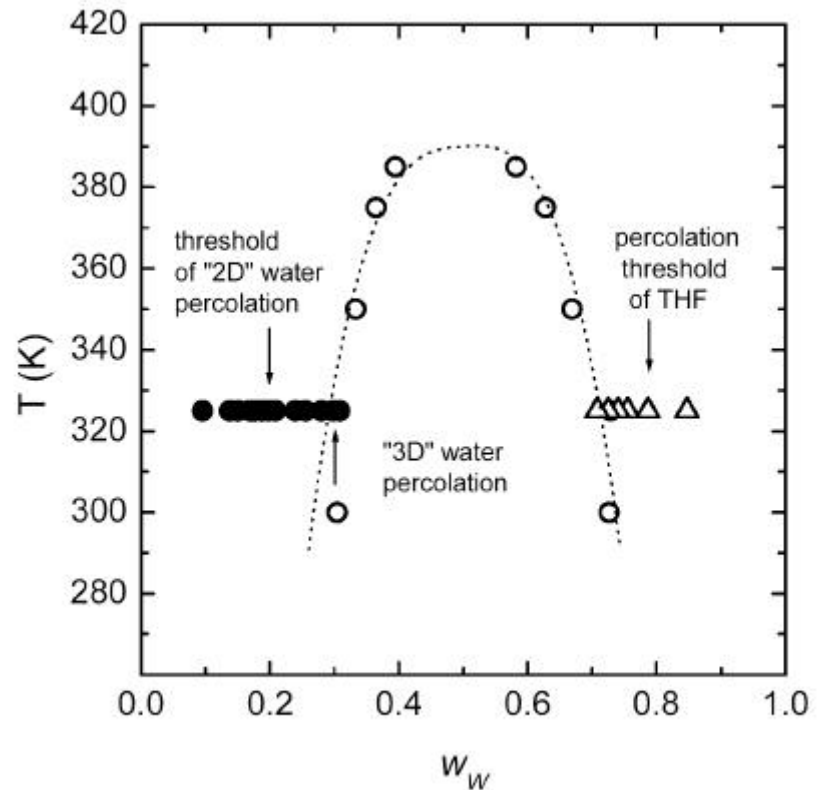
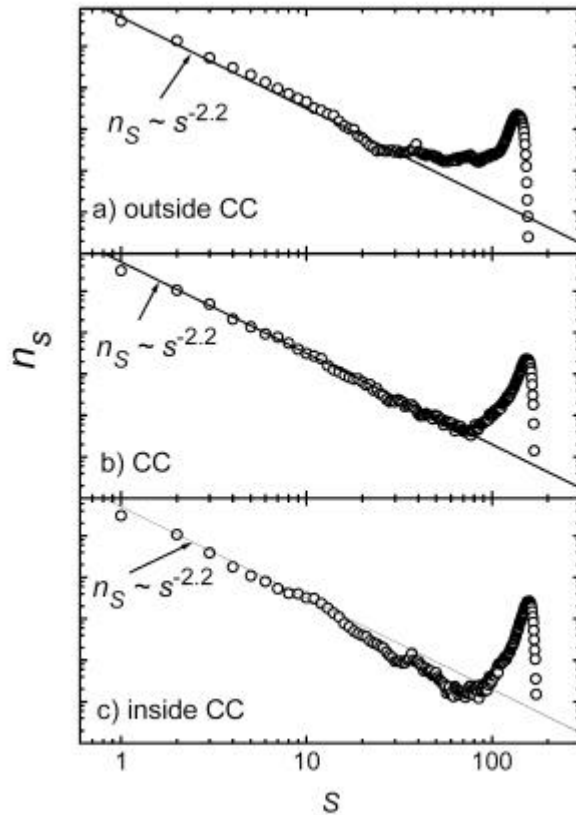


Phasendiagramm des adsorb. Wassers



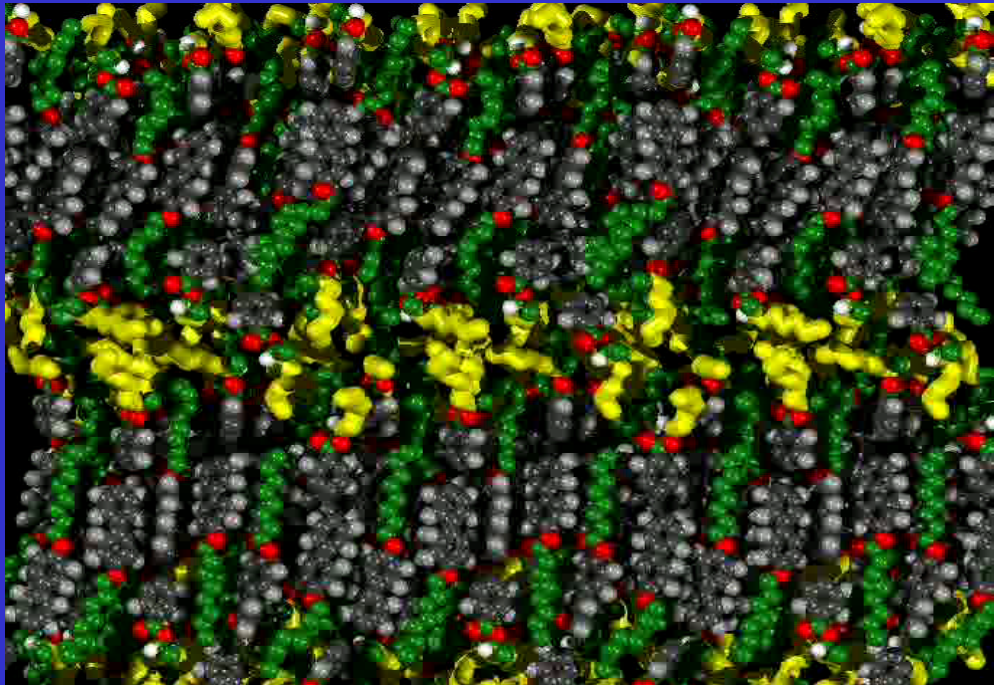
Vorhersage von Phasengleichgewichten

Perkulationsverhalten von Wasser/THF-Mischungen



Thermotrope Flüssigkristalle

Beispiel einer ferroelektrischen Flüssigkristall (FLC)-Phase

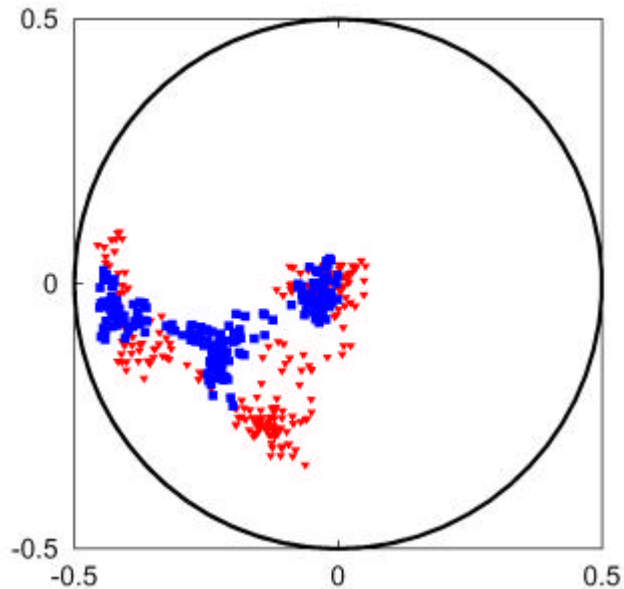


Molekül: MHPOBC; Phase: SmC*; T=375 K, p=1 atm

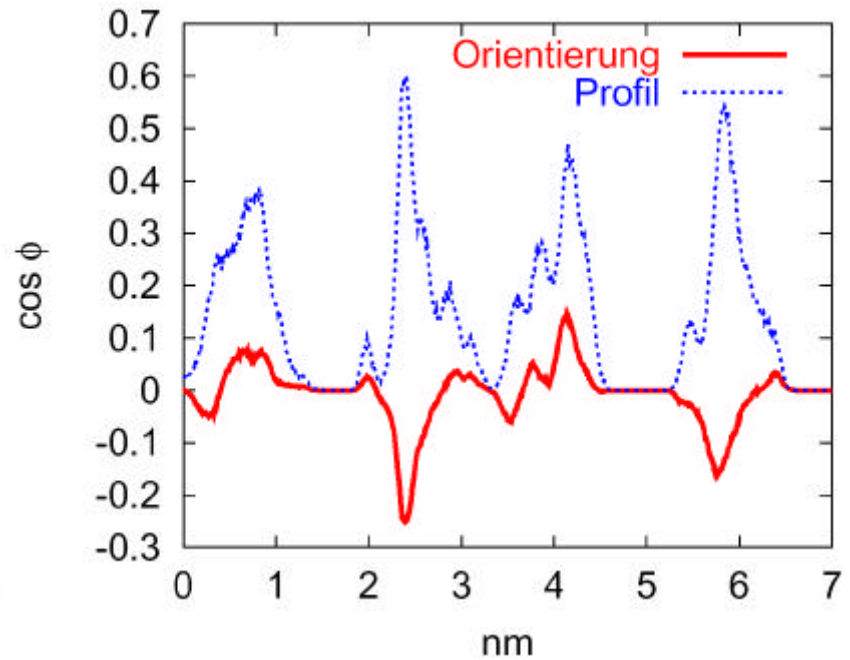
Antiferroelektrisches Verhalten; Sequenz: 12 ns

Orientierung der FLC-Moleküle

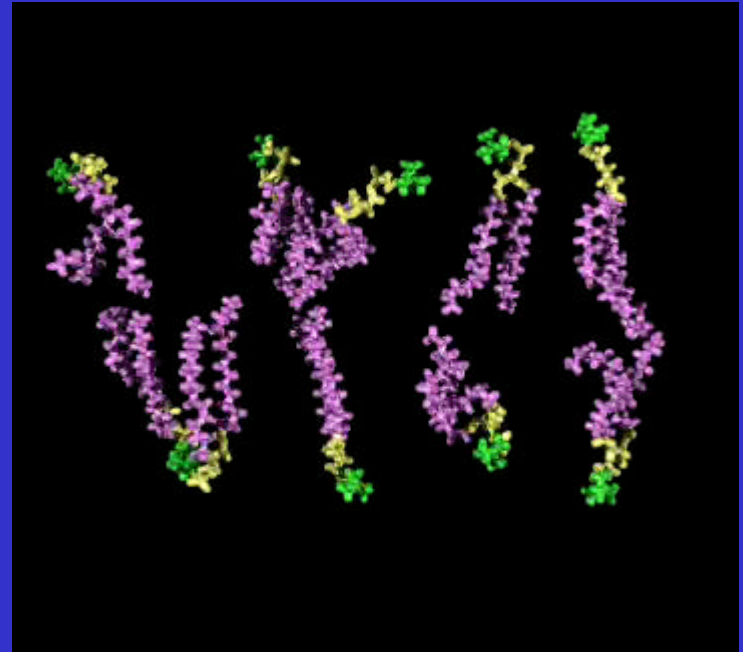
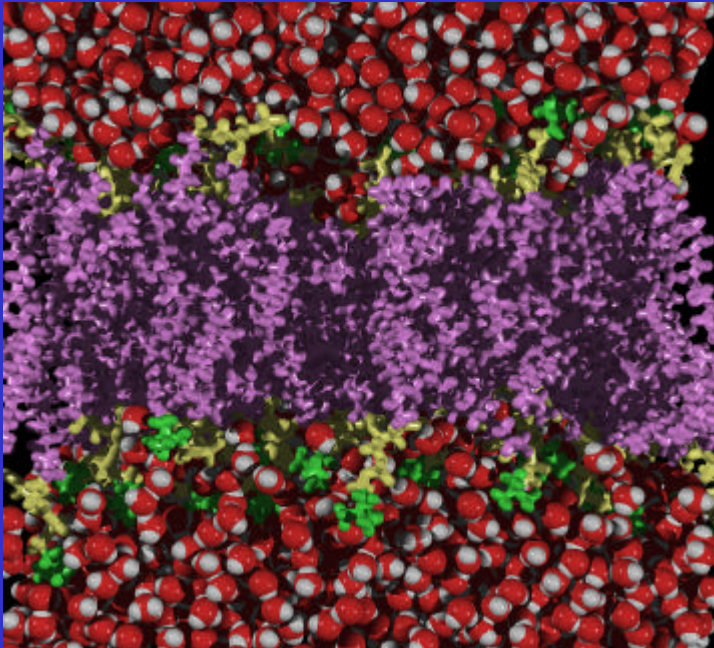
Orientierung des Direktors in beiden Schichten



Orientierung und Lage der CO-Gruppen



Hydratation biologischer Membranen

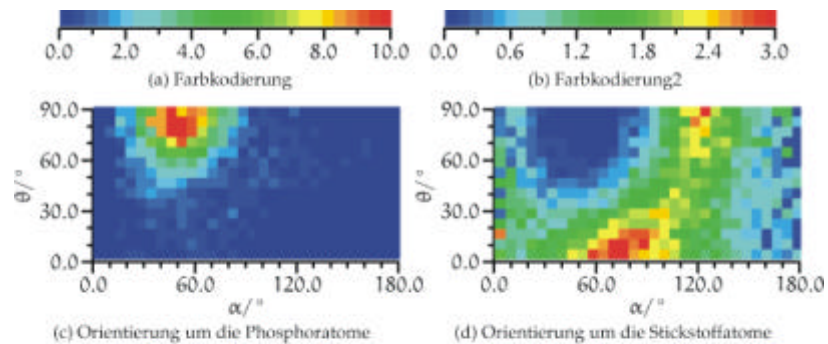


Voll hydratisierte DPPC (Dipalmitoyl-glycero-phosphatidylcholin)-Doppelschicht

Gel-Phase: Hohe Unordnung im Bereich der Alkylketten

T=330 K; p=1 atm; Sequenz: 6 ns

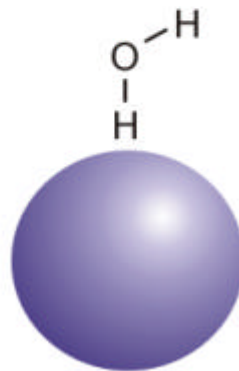
Orientierung des Hydrat-Wassers



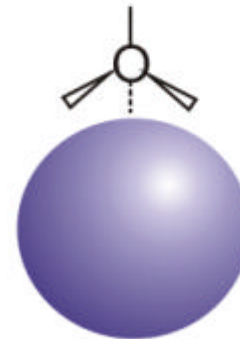
2d-Orientierungsverteilung

α : Dipol

θ : Molekülebenen-Normale

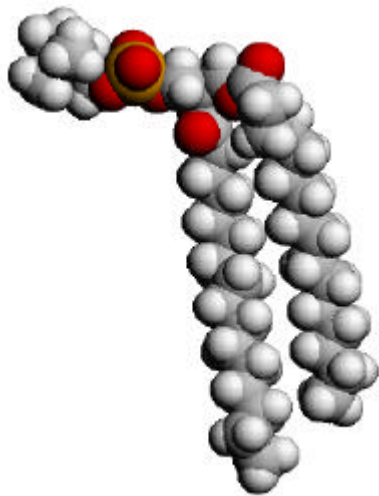


Anionisch



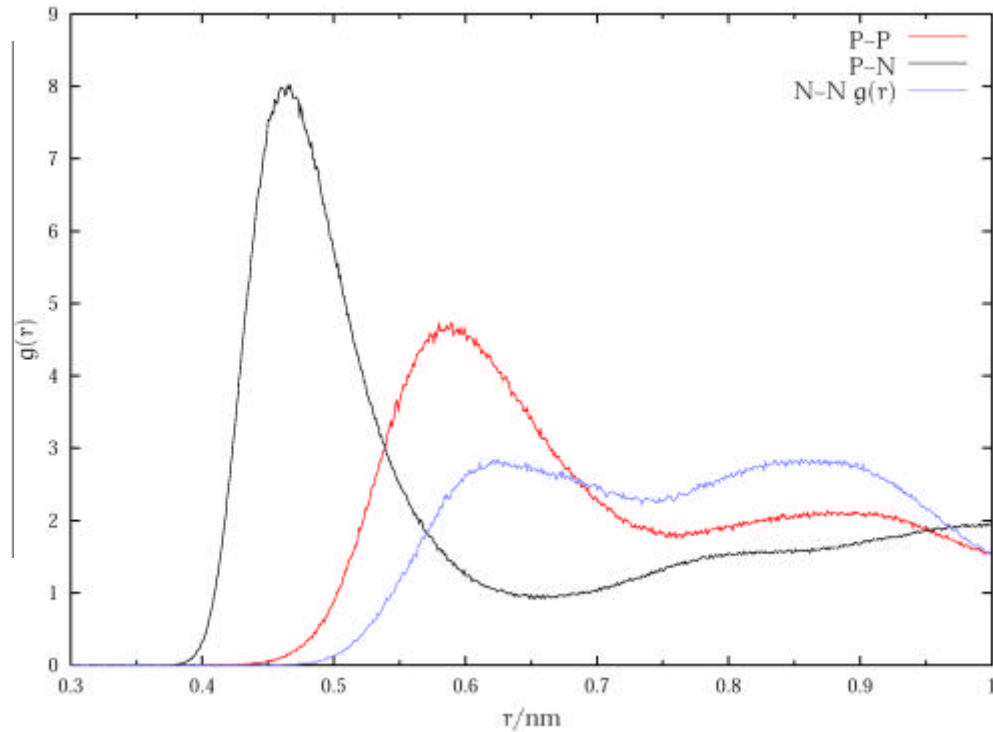
hydrophob

Orientierung der Kopfgruppen

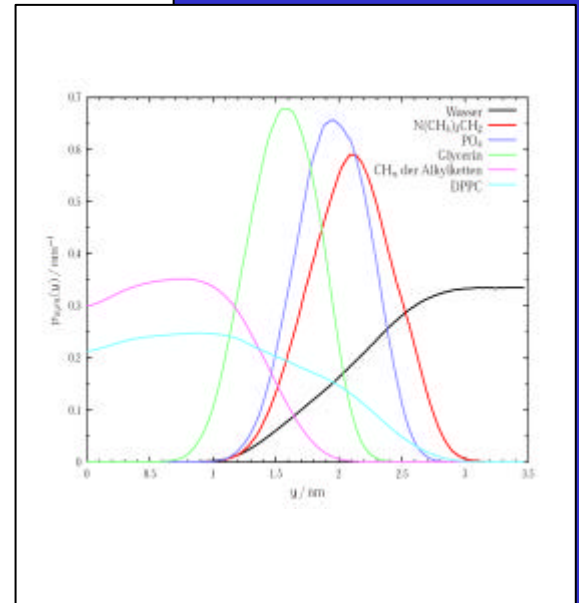
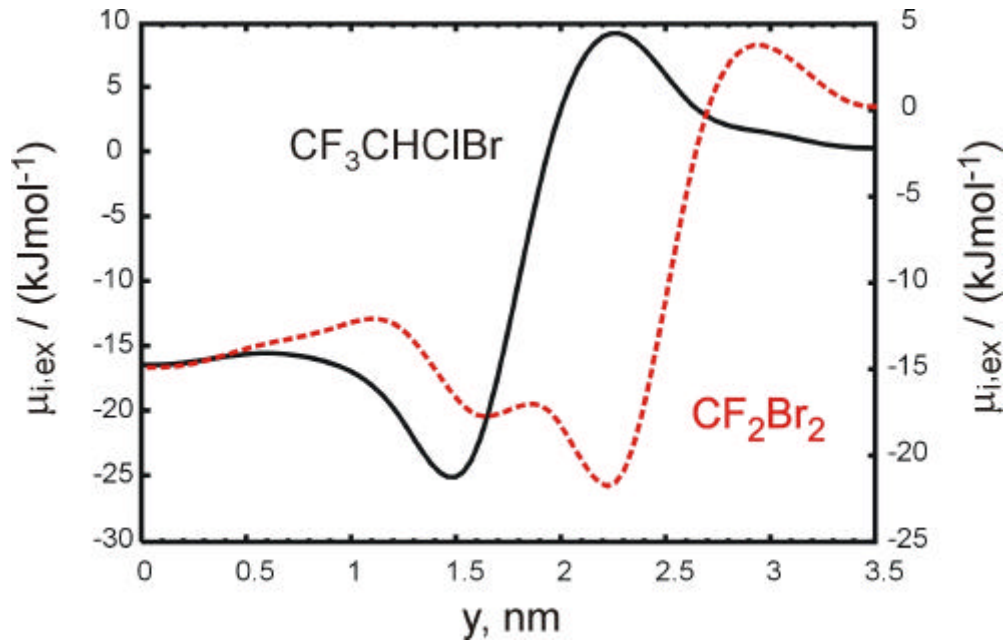


DPPC

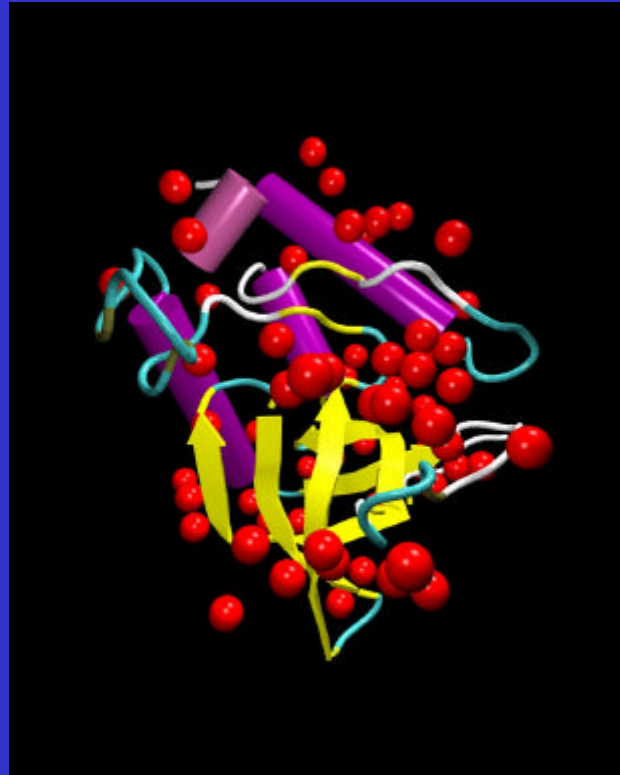
Atom-Atom-Paarverteilungsfunktionen



Einbau von Anästhetika in die Membran



Hydratationsverhalten von Proteinen

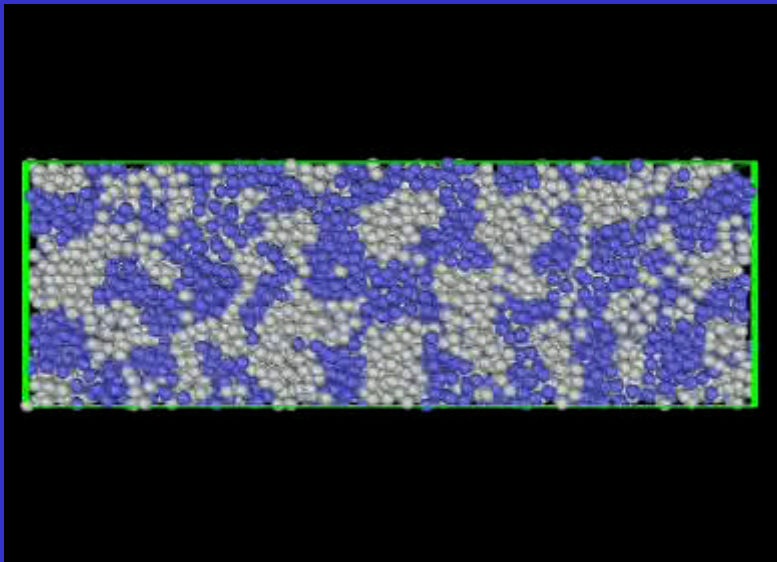


Struktur der hydratisierten S-Nase

MD-Simulation der druckinduzierten Denaturierung

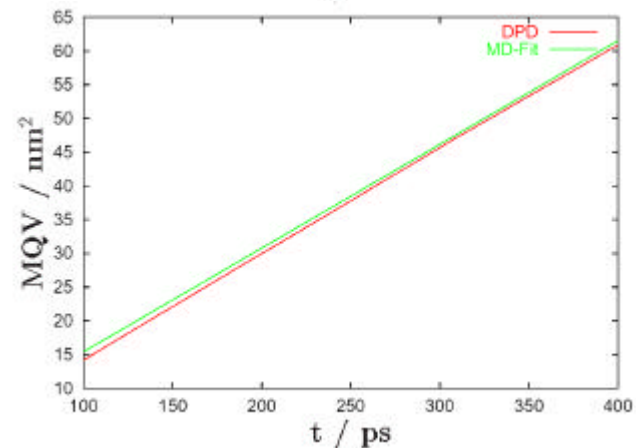
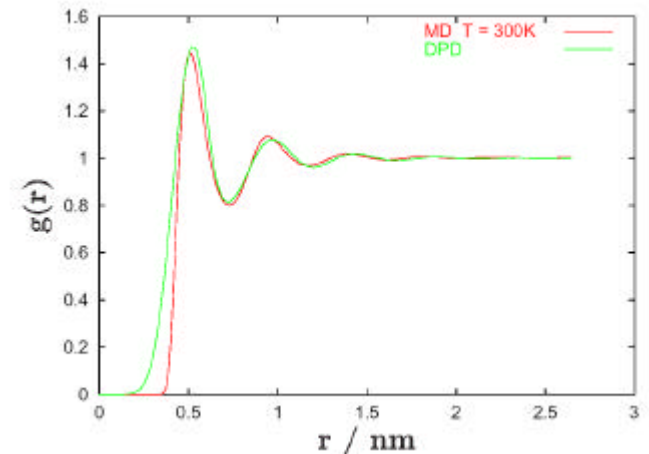
Mesoskopische Modelle

Entwicklung vereinfachter „coarse grained“ Dissipative Particle Dynamics (DPD)-Modelle



Mit DPD-Modellen ist ein größerer Zeitbereich zugänglich als mittels atomistischer MD. Aber unter Verlußt des atomaren Details.

Mapping der DPD-Parameter



Dank an:

Ralf Ludwig

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Ivan Brovchenko

Frank Schmauder

Ralf Schmelter

Nicolai Smolin

Sascha Nonn