Structure and Dynamics of Clathrate Hydrates

Christian Gutt

Werner Press

Mark Johnson

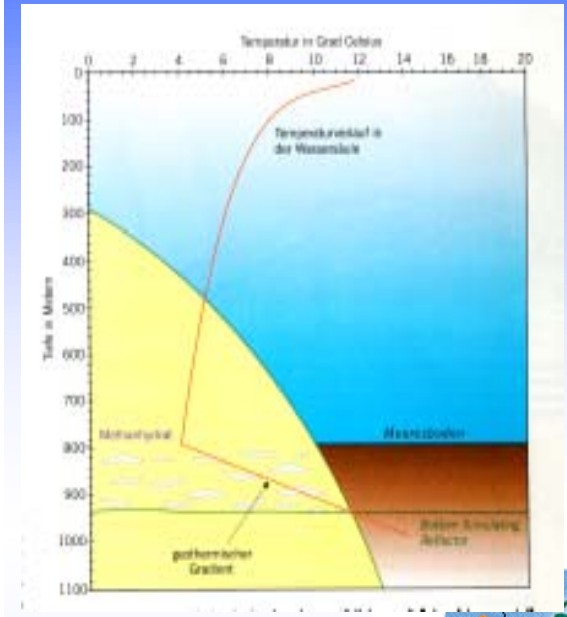
John S. Tse

National Research Council Canada / Conseil national de recherches Canada

Julian Baumert
ILL / University Kiel

GEOTECHNOLOGIEN

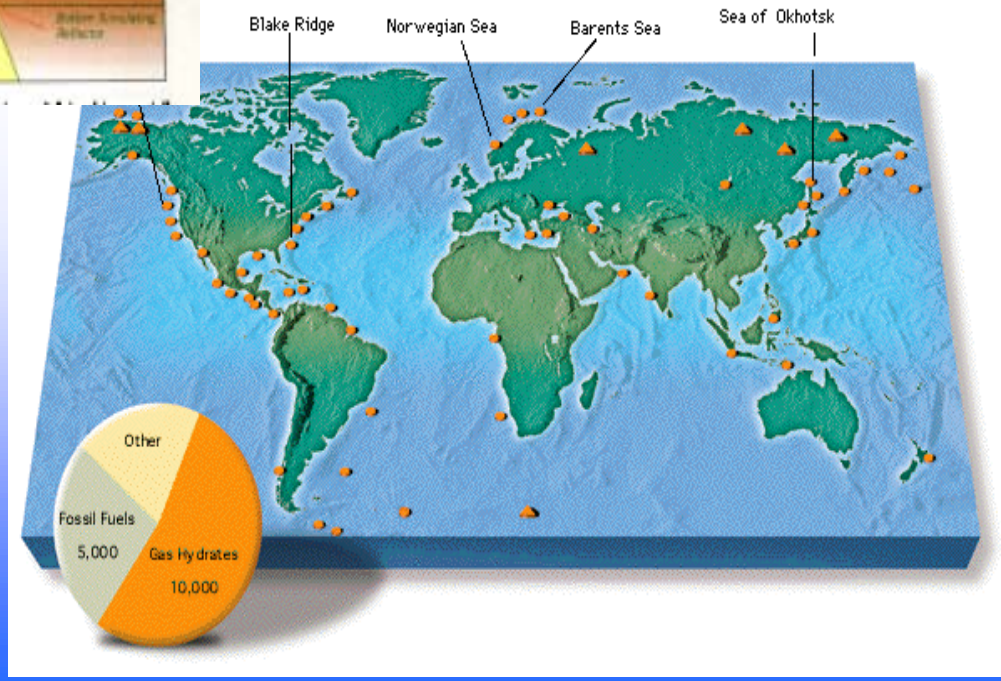
Natural Gas Hydrates



GEOMAR Kiel

Global Deposits

- Potential Energy Resource
- Greenhouse Gas



Projects and Methods

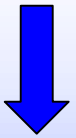
Structure

- **Diffraction under Natural Conditions (T=260-280 K, P=30-100 bar)**
- **Cage Deformations close to the Stability Limit**

Development of an optimised Sample Environment

Dynamics and Guest-Host Coupling

- **Density of State measured with Inelastic Neutron Scattering**
- **Velocity of Sound and Dispersion Relation**

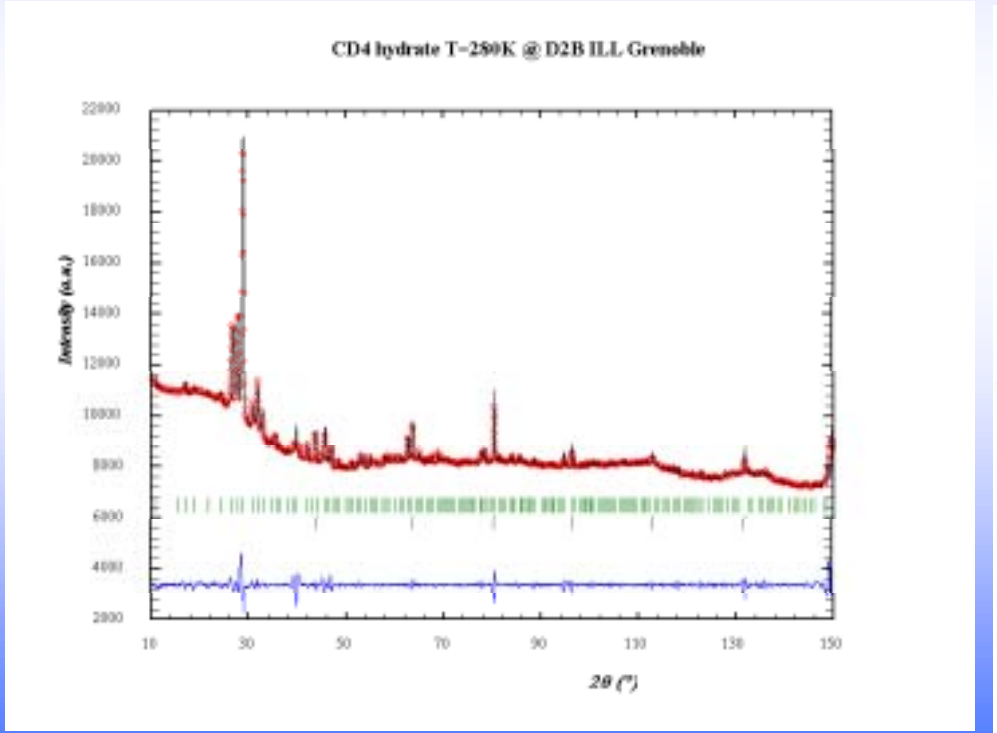


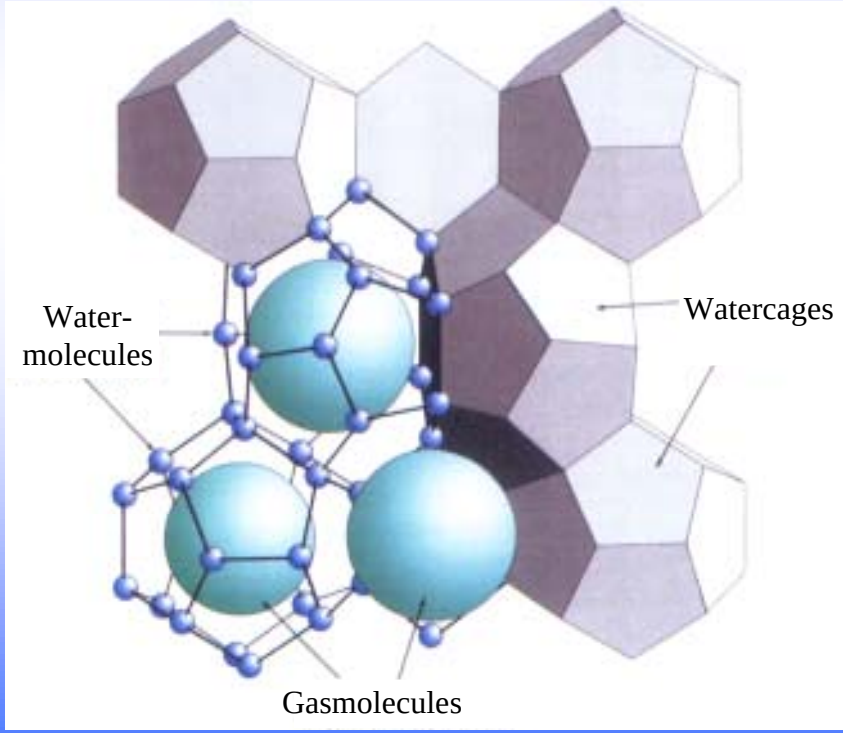
Explanations through Computational Modelling

Structure under Geological Conditions

Sample: CD_4 - D_2O Pressure: 100 bar

Temperature: 280 K



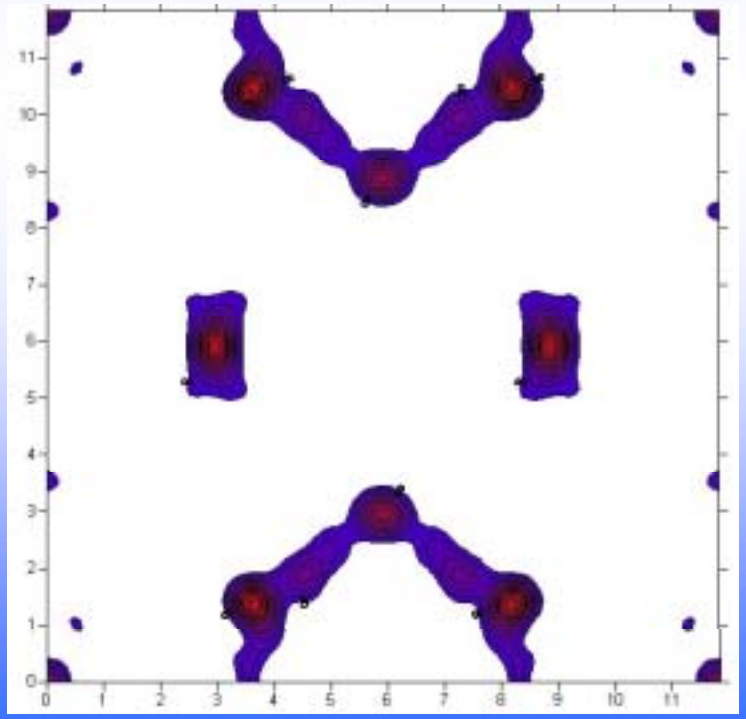


Structure under Geological Conditions

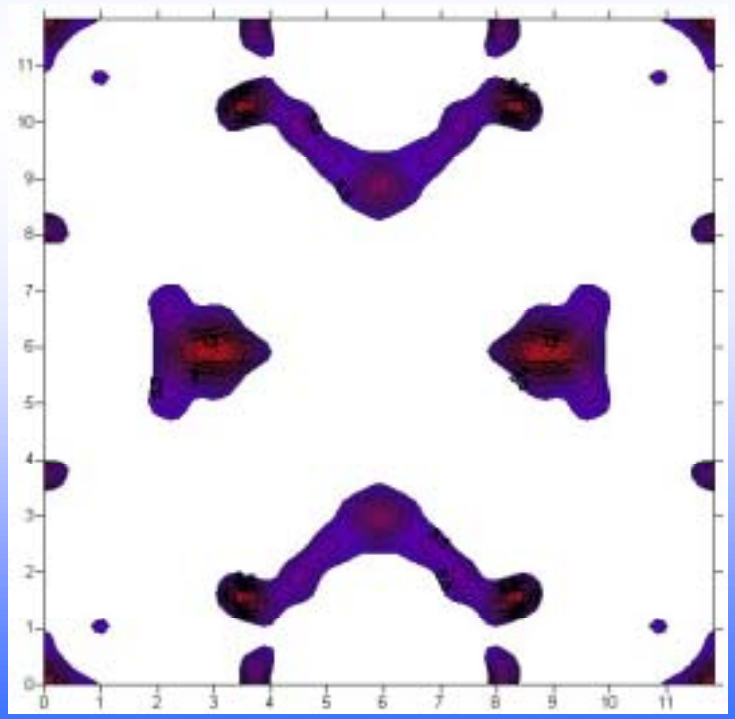
Sample: CD_4 - D_2O Pressure: 100 bar

Temperature: 280 K

T = 2 K

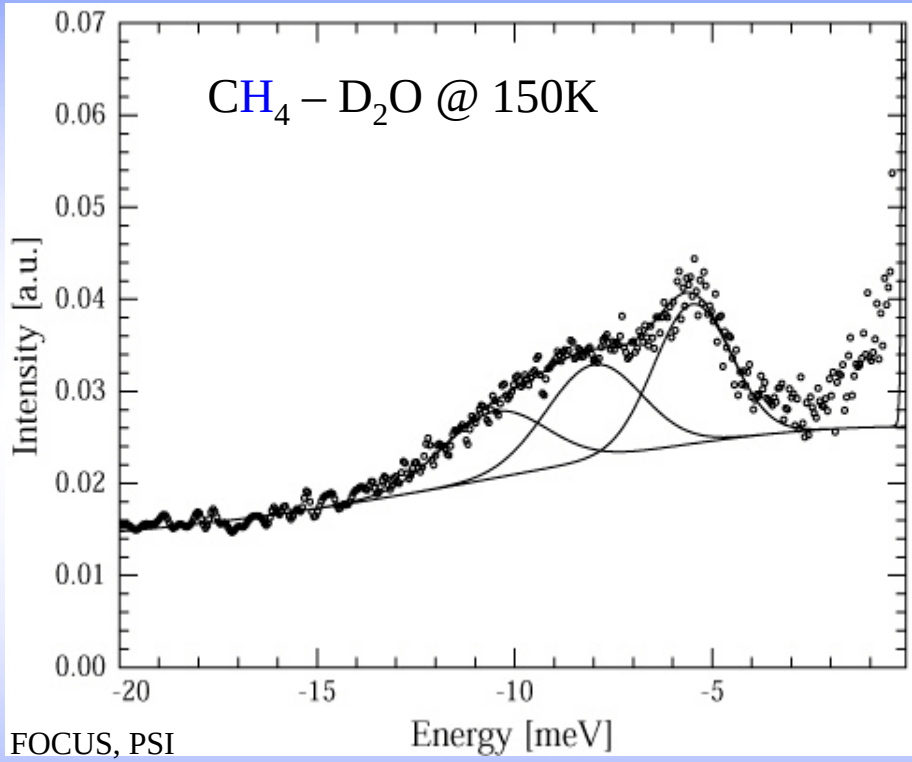


T = 280 K



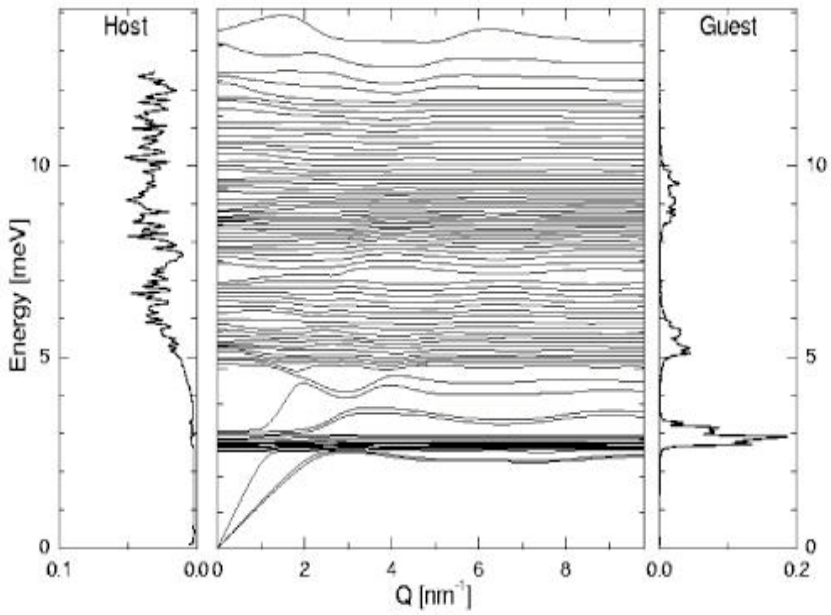
Guest-Host Coupling

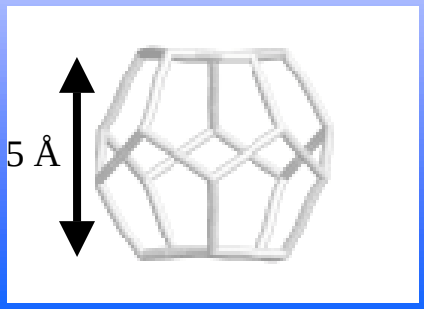
INS Experiment

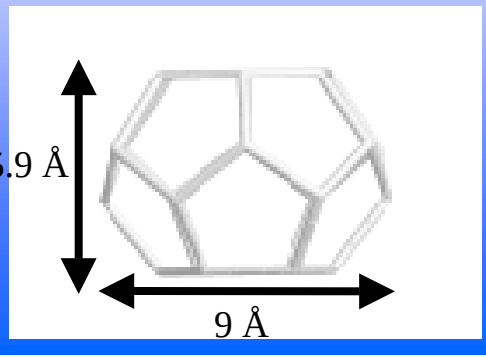


FOCUS, PSI

Lattice Dynamical Calculation

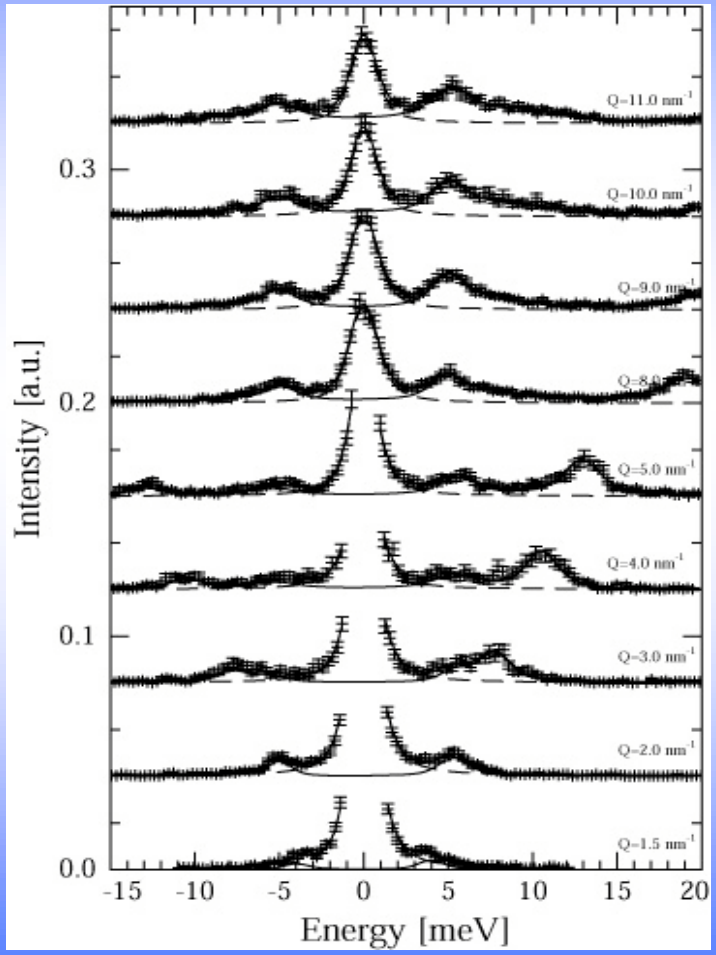




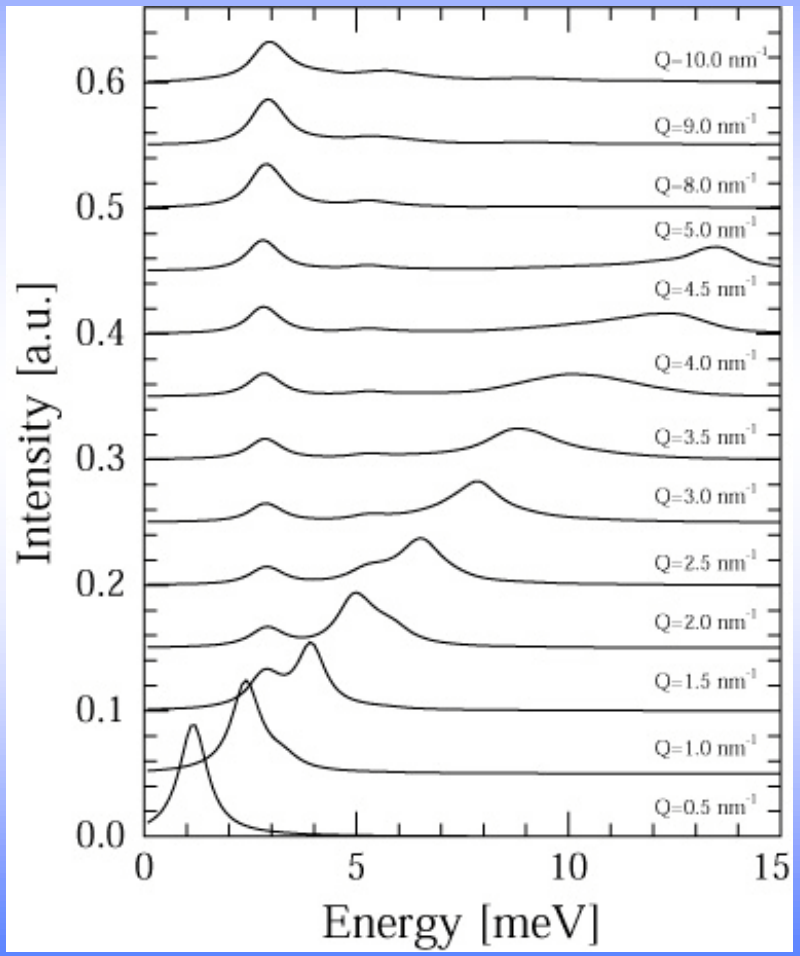


IXS Spectra of Methane Hydrate

IXS Experiment



Theor. IXS Spectra



Exp. Resolution: 0.75 meV

Theor. Resolution: 0.5 meV

Conclusions

Optimised Sample Environment

Structure

- **Diffraction under Natural Conditions (T=260-280 K, P=100 bar)**
- **Cage Deformations close to the Stability Limit**

Computational Modelling

Dynamics and Guest-Host Coupling

- **Density of State measured with Inelastic Neutron Scattering**
- **Velocity of Sound and Dispersion Relation measured with Inelastic X-Ray Scattering**