Research Center for Molecular Thermodynamics

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Structural Thermodynamics of Condensed Matter

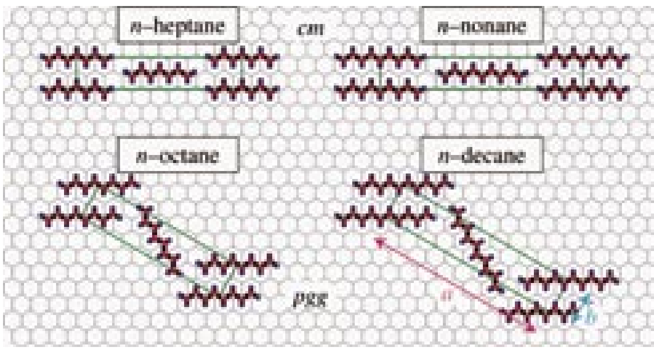
Our research covers a wide range of topics dealing with various types of condensed matter, including hard materials such as high-T_C superconductors, soft materials such as liquid crystals, and rather complex systems such as adsorbed monolayers. We are particularly interested in the order and disorder created by the subtle balance of various intermolecular interactions. The techniques that are employed to investigate the structure and dynamics are calorimetry, neutron scattering, X-ray diffraction, scanning probe microscopy and molecular dynamics simulation. Our specialty is to measure the energy and entropy very accurately. The goal is therefore to combine all the information obtained from both microscopic and macroscopic investigations to uncover the nature of condensed matter, which leads us to integrate molecular science and chemical thermodynamics.

1. Structure and thermodynamics of the two-dimensional solids formed at various interfaces
2. Structure and thermodynamics of quasicrystals, superconductors, and fullerenes
3. Thermodynamic behavior of novel glassy states including amorphous ices
4. Quantum effects and deuteration-induced phase transitions in hydrogen-bonded crystals
5. Thermodynamics of mesophases such as liquid crystals and plastic crystals
6. Thermodynamic investigation of molecular magnets and low-dimensional conductors
7. Energetics of biochemical systems including organisms

Details can be seen in our Annual Report at the URL above.

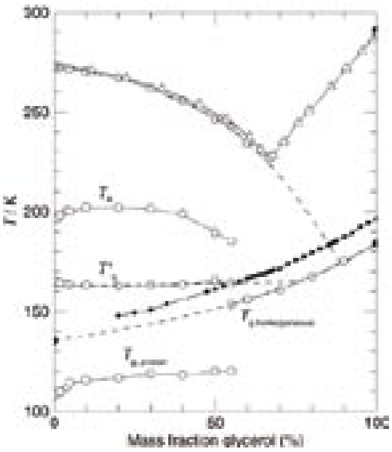
Two-Dimensional Solids at Interfaces

While molecular monolayers adsorbed on solid surfaces are both interesting and important in many ways, their detailed structure and dynamics, as well as their phase behavior, are difficult to investigate. Such investigations require probes that are sensitive enough to study the tiny quantities of material present in the adsorbed layers without the signals being dominated by the much larger quantities of bulk materials. The structure of adsorbed monolayers of pure linear alkanes was studied by X-ray and neutron diffraction. They exhibit a pronounced odd-even alternation in structure with alkyl chain length, particularly for the shorter members of the series.



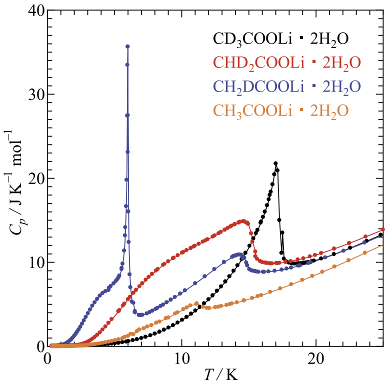
Non-Equilibrium Phase Diagram for Aqueous Solutions

Water–glycerol mixtures show a complex glass transition behavior for compositions in the range 0–55% (w/w) fraction glycerol that partly crystallizes on cooling. In this composition range, three glass transition-like anomalies occur on heating from 80 K. A low-temperature anomaly at about 115 K is due to the reorientational motion of the H_2O-molecules in hexagonal ice. On further heating, the vitrified liquid of maximally freeze-concentrated solution exhibits a glass transition at about 164 K. A third anomaly in the temperature drift rate and a step increase in the heat capacity occurs at about 200 K, most likely due to cold crystallization followed by ice dissolution, but a third glass transition cannot be completely ruled out.



Deuteration Induced Phase Transitions

The (partial) deuteration of a methyl group affects phase behavior substantially. For lithium acetate dihydrate, for example, the fully protonated sample shows the frozen-in phenomenon with the nuclear spin conversion, whereas the fully deuterated analog exhibits a phase transition at 17 K. Two partially deuterated analogs show complicated anomalies, reflecting successive orientational ordering of the methyl groups. Such a phenomenon illustrates a crossover from quantum to classical behavior caused by deuteration.



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