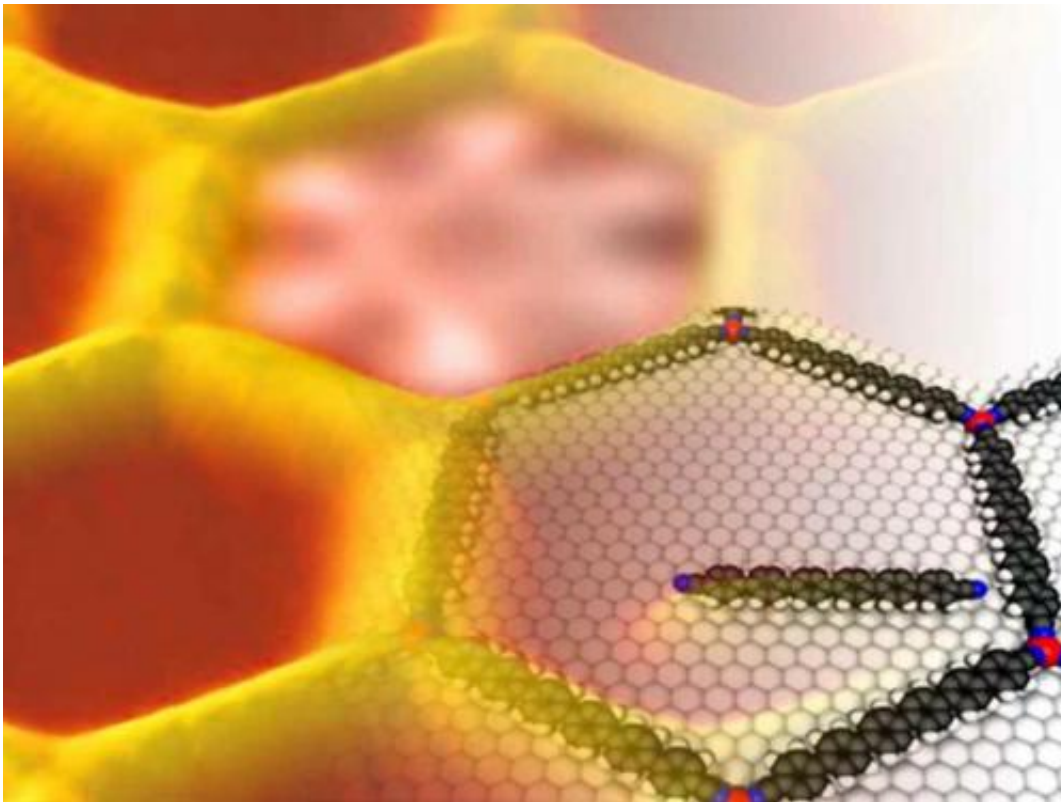


Caging of molecules allows investigation of equilibrium thermodynamics

February 26 2015



The nanopore restricts the the freedom of movement of the adsorbed single molecule thus enabling scientists at Technische Universitat Munchen and University Lingkoping to model the equilibrium thermodynamics of single molecules. Credit: Carlos-Andres Palma / TUM

High performance materials for gas storage, thermal insulators or nanomachines need a thorough understanding of the behavior of the

material down to the molecular level. Thermodynamics, which have been developed two hundred years ago to increase the efficiency of steam engines, typically observes and averages over a large number of molecules. Now a team of scientists has developed a methodology, to investigate the equilibrium thermodynamics of single molecules.

On the search for high performance materials for applications such as [gas storage](#), [thermal insulators](#) or dynamic nanosystems it is essential to understand the thermal behavior of matter down to the [molecular level](#). Classical [thermodynamics](#) average over time and over a large number of [molecules](#). Within a three dimensional space single molecules can adopt an almost infinite number of states, making the assessment of individual species nearly impossible.

Now researchers from Technische Universität München (TUM) and Linköping University (LIU) have developed a methodology, which allows to explore [equilibrium thermodynamics](#) of single molecules with atomic resolution at appreciable temperatures. The breakthrough study is based on two pillars: a technology which allows to cage molecules within two-dimensional nanopores and extensive computational modelling.

Trapped in two dimensions

At the Chair of Molecular Nanoscience and Chemical Physics of Interfaces at TU München, led by Prof. Dr. Johannes V. Barth, PD Dr. Florian Klappenberger developed the method to produce high-quality metal-organic networks on a silver surface. The network forms nanopores which restrict the freedom of movement of adsorbed single molecules in two-dimensions. Using scanning tunneling microscopy the researchers were able to track their motions at different temperatures with sub-nanometer resolution.

Parallel to the experiments, the researchers worked with sophisticated

computer models to describe the temperature dependence of the dynamics of these single trapped molecules. "We have applied state-of-the-art supercomputer calculations to understand the interactions and energy landscape determining the motion of the molecules", says Jonas Björk of Linköping University.

Comparing experimental and modeled data the scientists unraveled that under certain conditions the integral theory approaches a simple projection of the molecular positions in space. This approach is central to statistical mechanics, but has never before been challenged to reproduce an experiment, due to the practically infinite molecular positions and energies one needed to consider without the nanoscale confinement.

Analogy to biology

"It was extremely exciting to employ two-dimensional networks as a confinement strategy to reduce the available conformational space of a single molecule, like a chaperone does with a protein", says Dr. Carlos-Andres Palma, the lead author of the study. "In analogy to biology, such form of confinement technology has the potential to establish sensors, nanomachines and possibly logics controlled by and made of molecular distributions."

Applying their knowledge of characteristic equilibrium configurations, the researchers carefully modulated the nanopore, thus making a single molecule write letters of the alphabet such as L, I and U, just by fine-tuning the temperature.

Provided by Technical University Munich

Citation: Caging of molecules allows investigation of equilibrium thermodynamics (2015, February 26) retrieved 25 April 2024 from <https://phys.org/news/2015-02-caging-molecules-equilibrium-thermodynamics.html>

This document is subject to copyright. Apart from any fair dealing for the purpose of private study or research, no part may be reproduced without the written permission. The content is provided for information purposes only.