

Press Releases for JCP (2008-Current)

Public Release: 5-Oct-2010

■ The Journal of Chemical Physics

Model unfolds proteins gently

A new theoretical model reported in *The Journal of Chemical Physics* investigates the unfolding of the protein fibronectin under gentle conditions -- work that may lead to a better understanding of biomolecular transitions within the cell.

Pathways of mechanical unfolding of FnIII₁₀: Low force intermediates

M. Caraglio, A. Imparato, A. Pelizzola

J. Chem. Phys. **133**, 065101 (2010)

Public Release: 28-Sep-2010

■ The Journal of Chemical Physics

Finding a buckyball in photovoltaic cell

Research reported in *The Journal of Chemical Physics* describes a technique that analyzes the reflection of neutrons to locate buckyballs within composite materials. The work, conducted by scientists at the National Institute of Standards and Technology, may lead to more effective research on photovoltaic devices.

Phase-sensitive neutron reflectometry measurements applied in the study of photovoltaic films

J. W. Kiel, M. E. Mackay, B. J. Kirby, B. B. Maranville, and C. F. Majkrzak

J. Chem. Phys. **133**, 074902 (2010)

Public Release: 21-Sep-2010

■ The Journal of Chemical Physics

Watching electrons move in real time

Research published in *The Journal of Chemical Physics* describes the emerging technique of X-ray powder diffraction, which has been used to map the movement of electrons in real time and to observe a concerted electron and proton transfer that is quite different from any previously known phase transitions in the model crystal, ammonium sulfate.

Concerted electron and proton transfer in ionic crystals mapped by femtosecond x-ray powder diffraction

Michael Woerner, Flavio Zamponi, Zunaira Ansari, Jens Dreyer, Benjamin Freyer, Mirabelle Premont-Schwarz, and Thomas Elsaesser

J. Chem. Phys. **133**, 064509 (2010)

Public Release: 14-Sep-2010

■ The Journal of Chemical Physics

How do your crystals grow?

Research reported in *The Journal of Chemical Physics* uses fluorescence correlation spectroscopy to investigate the processes at the surface of a growing crystal. This work may help to improve the crystallization of biomolecules -- an important tool in pharmaceutical research and other fields.

Slow molecular dynamics close to crystal surfaces during crystallization of a protein lysozyme studied by fluorescence correlation spectroscopy

Shinpei Tanaka

J. Chem. Phys. **133**, 095103 (2010)

Public Release: 3-Aug-2010

■ The Journal of Chemical Physics

Molecules delivering drugs as they walk

A new paper in *The Journal of Chemical Physics* provides a theoretical model that compares the transport characteristics of straight- and branched-chain polymers in various channels -- work that could aid in the development of carrier molecules for delivering drugs at a controlled rate in the body.

Flow-induced polymer translocation through narrow and patterned channels

Arash Nikoubashman and Christos Likos

J. Chem. Phys. **133**, 074901 (2010)

Public Release: 27-Jul-2010

■ The Journal of Chemical Physics

Artificially controlling water condensation leads to 'room-temperature ice'

Researchers in Spain have studied the underlying mechanisms of water condensation in the troposphere and found a way to make artificial materials to control water condensation and trigger ice formation at room temperature -- all described in *The Journal of Chemical Physics*.

Two-dimensional wetting: The role of atomic steps on the nucleation of thin water films on BaF₂(111) at ambient conditions

M. Cardellach, A. Verdaguer, J. Santiso, and J. Fraxedas

J. Chem. Phys. **132**, 234708 (2010)

Public Release: 27-Jul-2010

■ The Journal of Chemical Physics

Where do the drugs go?

Drug delivery inside the body is a complicated process. Compounds travel through a maze of aqueous solutions, lipid membranes, and barriers between the blood and tissues like the brain.

Accurate calculations of the hydration free energies of druglike molecules using the reference interaction site model

David S. Palmer, Volodymyr P. Sergiievskiy, Frank Jensen, and Maxim V. Fedorov

J. Chem. Phys. **133**, 044104 (2010)

Public Release: 21-Jul-2010

■ The Journal of Chemical Physics

Quantum entanglement in photosynthesis and evolution

Recently, academic debate has been swirling around the existence of unusual quantum mechanical effects in the most ubiquitous of phenomena, including photosynthesis, the process by which organisms convert light into chemical energy. In a paper in *The Journal of Chemical Physics*, these ideas are put to the test.

Quantum oscillatory exciton migration in photosynthetic reaction centers

Darius Abramavicius and Shaul Mukamel

J. Chem. Phys. **133**, 064510 (2010)

Public Release: 13-Jul-2010

■ The Journal of Chemical Physics

[A simple quantum dynamics problem?](#)

Research reported in *The Journal of Chemical Physics*, which is published by the American Institute of Physics, provides the first real-time measurements of the time dependence of the individual steps of dissociation of a complex consisting of two rare gas atoms and a halogen molecule.

Real-time dissociation dynamics of the Ne₂Br₂ van der Waals complex

Jordan M. Pio, Molly A. Taylor, Wytze E. van der Veer, Craig R. Bieler, Jose A. Cabrera, and Kenneth C. Janda

[J. Chem. Phys. 133, 014305 \(2010\)](#)

Public Release: 13-Jul-2010

■ The Journal of Chemical Physics

[Moving polymers through pores](#)

The movement of long chain polymers through nanopores is a key part of many biological processes, including the transport of RNA, DNA, and proteins. New research reported in *The Journal of Chemical Physics* describes an improved theoretical model for this type of motion.

Polymer translocation through pores with complex geometries

Aruna Mohan, Anatoly B. Kolomeisky, and Matteo Pasquali

[J. Chem. Phys. 133, 024902 \(2010\)](#)

Public Release: 29-Jun-2010

■ The Journal of Chemical Physics

[Fast-tracking the manufacture of glasses](#)

Old glass is not the same as new glass -- and the difference is not just due to manufacturing techniques. Unlike crystalline solids, glasses change as they age, increasing packing density and stability. Ideally, a glass should be cooled slowly, maybe over 10,000 years or so, but that is not usually practical. Research reported in *The Journal of Chemical Physics* details the production of highly stable glass films of indomethacin by physical vapor deposition.

Observation of low heat capacities for vapor-deposited glasses of indomethacin as determined by AC nanocalorimetry

Kenneth L. Kearns, Katherine R. Whitaker, M. D. Ediger, Heiko Huth, and Christoph Schick

[J. Chem. Phys. 133, 014702 \(2010\)](#)

Public Release: 22-Jun-2010

■ The Journal of Chemical Physics

[Report describes the physics of the 'bends'](#)

As you go about your day-to-day activities, tiny bubbles of nitrogen come and go inside your tissues. This is not a problem unless you happen to experience large changes in pressure, as scuba divers and astronauts may. During large, fast pressure drops, bubbles can grow, causing "the bends." A study in *The Journal of Chemical Physics* may provide a physical basis for the existence of these bubbles and help explain decompression sickness.

Free energy wells for small gas bubbles in soft deformable materials

Saul Goldman

[J. Chem. Phys. 132, 164509 \(2010\)](#)

Public Release: 16-Jun-2010

■ The Journal of Chemical Physics

The secret life of water at very low temperatures

The secret life of water just got weirder. For years water has been known to exist in 15 phases -- not just the merry threesome of solid, liquid and gas from grade school science. Now, University of Utah chemists have confirmed the coexistence of ice and liquid after water crystallizes at very low temperatures. They describe their work in *The Journal of Chemical Physics*, which is published by the American Institute of Physics.

Ice crystallization in water's "no-man's land"

Emily Moore and Valeria Molinero

J. Chem. Phys. **132**, 244504 (2010)

Public Release: 16-Jun-2010

■ The Journal of Chemical Physics

Geometry affects drift and diffusion across entropic barriers

Understanding particle diffusion in the presence of constrictions is essential in fields as diverse as drug delivery, cellular biology, nanotechnology, materials engineering, and spread of pollutants in the soil. When a driving force is applied, displacement of particles occurs as well as diffusion. A paper in *The Journal of Chemical Physics* published by the American Institute of Physics, quantifies the effects of periodic constrictions on drift and diffusion in systems experiencing a driving force.

Communications: Drift and diffusion in a tube of periodically varying diameter. Driving force induced intermittency

Alexander M. Berezhkovskii, Leonardo Dagdug, Yurii A. Makhnovskii, and Vladimir Yu. Zitserman

J. Chem. Phys. **132**, 221104 (2010)

Public Release: 29-Apr-2009

■ The Journal of Chemical Physics

Simulated gene therapy

In a recent issue of *The Journal of Chemical Physics*, published by the American Institute of Physics, a group of researchers at the University of California, Berkeley and Los Alamos National Laboratory describe the first comprehensive, molecular-level numerical study of gene therapy. Their work should help scientists design new experimental gene therapies and possibly solve some of the problems associated with this promising technique.

Dendrimers as synthetic gene vectors: Cell membrane attachment

N. K. Voulgarakis, K. Ø. Rasmussen, and P. M. Welch

J. Chem. Phys. **130**, 155101 (2009)

Public Release: 14-Apr-2009

■ The Journal of Chemical Physics

Next generation nanofilms created -- new research described in AIP's *The Journal of Chemical Physics*

With the human genome in hand, biochemists have cataloged the 3-D structures of thousands of proteins isolated from living cells. But one important class of proteins -- those stuck in the cell membranes -- has proven difficult to extract and study in 3-D crystals. Now an international team of scientists has developed a way to train such molecules to line up neatly on the surface of water in thin, tissue-like layers called nanofilms.

Laser-induced aligned self-assembly on water surfaces

Iftach Nevo, Sergey Kapishnikov, Atalia Birman, Mingdong Dong, Sidney R. Cohen, Kristian Kjaer, Flemming Besenbacher, Henrik Stapelfeldt, Tamar Seideman, and Leslie Leiserowitz

J. Chem. Phys. **130**, 144704 (2009)

Public Release: 25-Nov-2008

■ The Journal of Chemical Physics

New discovery may enhance MRI scans, lead to portable MRI machines

Researchers in Ohio and France have solved a longstanding scientific mystery involving magnetic resonance -- the physical phenomenon that allows MRI instruments in modern hospitals to image tissues deep within the human body. Their discovery, a new mathematical algorithm, should lead to new MRI techniques with more informative and sharper images.

Superadiabaticity in magnetic resonance

Michaël Deschamps, Gwendal Kervern, Dominique Massiot, Guido Pintacuda, Lyndon Emsley, and Philip J. Grandinetti

J. Chem. Phys. **129**, 204110 (2008)