COVER
Simulation of a vesicle interacting with a lipid bilayer (lipid head groups in green and blue, tails in cyan; water is not shown). The computation uses a coarse-grained model with over 1 million interaction sites, equivalent to more than 10 million atoms. See the special section beginning on page 783.

Image: Wataru Shinoda/Research Institute for Computational Sciences, National Institute of Advanced Industrial Science and Technology, Japan; Mike Klein/Center for Molecular Modeling, University of Pennsylvania

SPECIAL SECTION
Challenges in Theoretical Chemistry

INTRODUCTION
Theoretical Possibilities  783

NEWS
Problem Solved* (*Sort Of)  784

PERSPECTIVES
Intermolecular Potentials  787
A. J. Stone
Quantum Dynamics of Chemical Reactions  789
D. C. Clary
Insights into Current Limitations of Density Functional Theory  792
A. J. Cohen et al.
Frontiers in Surface Scattering Simulations  794
G.-J. Kroes
Large-Scale Molecular Dynamics Simulations of Self-Assembling Systems  798
M. L. Klein and W. Shinoda
Challenges in Modeling Materials Properties Without Experimental Input  800
E. A. Carter

NEWS OF THE WEEK
Scientists Seek Answers, Ponder Future After Anthrax Case Suicide  754
Scientists Targeted in California Firebombings  755
Court Ruling Scrambles Clean Air Plans, Leaving a Vacuum  756
Ethics Questions Add to Concerns About NIH Lines  756

SCIENCESCOPE
Phoenix’s Water May Be Gumming Up the Works  758
Successes, Past and Future  759

NEWS FOCUS
Deciphering the Genetics of Evolution  760
Industrial-Style Screening Meets Academic Biology  764
Universities Join the Screening Bandwagon
Can the Vaquita Be Saved?  767
ATMOSPHERIC SCIENCE
Atmospheric Warming and the Amplification of Precipitation Extremes
R. P. Allan and B. J. Soden
Satellite data show that in the tropics, heavy rain events have increased in warmer months and decreased in colder months, more than predicted by climate models.
10.1126/science.1160787

BIOCHEMISTRY
Helical Structures of ESCRT-III Are Disassembled by VPS4
S. Lata et al.
A protein responsible for the final separation of daughter cells or budding viruses forms heteromeric complexes on the inside of the membrane to regulate the abscission step.
10.1126/science.1161070

EVOLUTION
Parasite Treatment Affects Maternal Investment in Sons
T. E. Reed et al.
Mother seabirds that are infected by parasitic nematodes are less able to gather food and feed their fast-growing sons, shifting the sex ratio and affecting population viability.
10.1126/science.1159466

LETTERS
The Drugs Not Taken J. Urquhart 769
The Potential of Genotyping J. De Leon
Correcting the Record on DNA Direct A. T. Bombard and T. Brown Response S. Katsanis et al.
Blue Revolution Brings Risks and Rewards D. A. Lightfoot
Bad Grades for Science Title J. H. Marburger III

CORRECTIONS AND CLARIFICATIONS 772

BOOKS ET AL.
Plague and the End of Antiquity The Pandemic of 541–750 L. K. Little, Ed.; Pestilian Complexities Understanding Medieval Plague V. Nutton, Ed.; reviewed by N. Ch. Stenseth
What the Nose Knows The Science of Scent in Everyday Life A. Gilbert, reviewed by S. Firestein

POLICY FORUM
Scientific Misconduct: Do the Punishments Fit the Crime? B. K. Redman and J. F. Merz

PERSPECTIVES
A Breath of Aire for the Periphery B. Kyewski 776
Planetary System Formation J. C. B. Papaloizou 777
Trust Me on This A. Meyer-Lindenberg 778
The Coming Arctic Invasion G. J. Vermeij and P. D. Roopnarine 780
Symmetric Transporters for Asymmetric Transport N. K. Karpowich and D.-N. Wang 781

BREVIA
CHEMISTRY
Imaging of fingerprints in the field with a portable mass spectrometer can reveal the presence of drugs, explosives, or other materials and help resolve overlapping prints.
10.1126/science.1160309

RESEARCH ARTICLES
PSYCHOLOGY
The Rupture and Repair of Cooperation in Borderline Personality Disorder B. King-Casas et al.
In a game, patients with personality disorder cannot build trust with normal partners, possibly because they cannot distinguish between trusting and distrusting acts in others.
>> Perspective p. 778; Science Podcast

BIOCHEMISTRY
The Crystal Structure of a Sodium Galactose Transporter Reveals Mechanistic Insights into Na+/Sugar Symport S. Faham et al.
The structure of a sugar transporter suggests how these proteins may rearrange to permit the sugar to enter and leave the binding site on opposite sides of the membrane. >> Perspective p. 781

ASTRONOMY
A model of the evolution of planets from a gas-rich disk shows that the disk’s density and viscosity affect the final distribution of planets and that our solar system is unusual. >> Perspective p. 777

777 & 814

Published by AAAS on July 14, 2017

http://science.sciencemag.org/
EVOLUTION
A Conserved Mutation in an Ethylene Biosynthesis Enzyme Leads to Andromonoecy in Melons
A. Boualem et al.
Melon plants have both hermaphroditic and male flowers, a mating system that results from a mutation involved in ethylene synthesis that is still under positive selection.

MEDICINE
Human CHN1 Mutations Hyperactivate α2-Chimaerin and Cause Duane’s Retraction Syndrome
N. Miyake et al.
A signaling protein that helps nerve fibers find their correct target muscles is required for innervation of the eye muscles and, if defective, causes an eye movement disorder.

IMMUNOLOGY
Deletional Tolerance Mediated by Extrathymic Aire-Expressing Cells
J. M. Gardner et al.
Cells in the spleen and lymph nodes express self-antigens to detect and remove circulating self-reactive immune cells that have escaped deletion by the thymus.

NEUROSCIENCE
Dynamic Shifts of Limited Working Memory Resources in Human Vision
P. M. Bays and M. Husain
Working memory is a flexibly allocated, but finite, resource; more attention given to an object means it is remembered more precisely, whereas other objects are remembered less well.

ATMOSPHERIC SCIENCE
Brown Carbon Spheres in East Asian Outflow and Their Optical Properties
D. T. L. Alexander, P. A. Crozier, J. R. Anderson
Pollution blown from East Asia over the Pacific contains abundant brown spheres, not simply black or organic carbon particles, complicating modeling of its climatic effects.
In contrast to its stolid image, the Z band of the mature myofibril is a beehive of activity.

**FUNDING SOURCES**
Browse a list of grants and funding opportunities for cell signaling research and training; in the Resources section.

---

**SCIENCE NOW**
www.sciencenow.org
HIGHLIGHTS FROM OUR DAILY NEWS COVERAGE

**Poached Tusks Point to Killing Fields**
Genetic analysis enables researchers to trace contraband to region of origin.

**Unmasking Dark Energy**
Astronomers find its unseen hand at work in the biggest structures in the universe.

**Stem Cell Breakthrough in ALS Research**
Researchers reprogram skin cells from a patient to become motor neurons.

---

**SCIENCE CAREERS**
www.sciencecareers.org/career_development
FREE CAREER RESOURCES FOR SCIENTISTS

**Science Careers Podcast: Geoscience Careers**
*K. Travis*
Hear from experts and geologists about the current job market for geoscientists.

>> See also Geoscience Careers feature p. 856

---

**SCIENCE PODCAST**
www.sciencemag.org/multimedia/podcast
FREE WEEKLY SHOW

Download the 8 August Science Podcast to hear about science in Muslim countries, the brain signature of borderline personality disorder, geoscience careers, and more.

---

Separate individual or institutional subscriptions to these products may be required for full-text access.
Science 321 (5890), 741-859.