



Telephone-wire basket
by Anna Maria Dlamini.

BIOMEDICINE

To Have or Have Not

The rollout of antiretroviral therapy during 2004–2008 in South Africa brings with it severe ethical dilemmas regarding the allocation of drugs, because supply will outstrip need. Incorporating data from KwaZulu-Natal in a spatially explicit mathematical model, Wilson *et al.* have applied the government's allocation strategy in three scenarios to predict the consequences of different choices.

The modeling reveals clearly that for preventing transmission, the most effective strategy is to concentrate all of the doses (for half a million people living with HIV) in Durban, where HIV prevalence is 13%. This will have the effect of preventing 15,000 infections by 2008, minimizing the transmission of drug resistance, and preventing the greatest number of deaths. But this choice is not egalitarian, and the intent of antiretroviral therapy is treatment and not prevention. However, if the drug allocation were split between urban and rural areas (just over half of the KwaZulu-Natal population is rural, with an HIV prevalence of 9%), its effectiveness for HIV prevention would be reduced by about a third to a half, not just because the rural population is dispersed but also because the rural health infrastructure is relatively weak and because distribution and clinical monitoring will not be so effective. — CA

Proc. Natl. Acad. Sci. U.S.A. **103**, 14228 (2006)

PSYCHOLOGY

Saving Face

It is well established that the perception of probabilities can be influenced by how a particular likelihood is framed or anchored, and that the consequences for a patient if the number qualifies a medical prognosis can be real and serious. Bonnefon and Villejoubert propose another context in which the diagnosis of a possible condition is not perceived to reflect its likelihood but instead is taken as warning of a dire outcome. Upon quizzing subjects (recruited by and not representative of psychology students) after a physician had delivered an assessment of possible insomnia or deafness, they found that the condition regarded as more serious (deafness) was judged to be more likely to occur and that the use of the word possible was interpreted as a means of softening the news. In contrast, subjects who adhered to a probabilistic interpretation of the phrasing believed that both conditions were equally likely outcomes, underlining the importance of mutual understanding in physician-patient discussions. — GJC

Psychol. Sci. **17**, 747 (2006).

CHEMISTRY

Twisting with Fewer Breaks

In polymer synthesis, chiral solvents can be used to increase the stereoregularity, or tacticity, of polymer chains. However, in the synthesis of some polymers, the alternation between helical senses also affects the distribution of chain lengths.

Holder *et al.* point out that in the Wurtz-type reductive coupling of dichloro-diorganosilanes to form polymers on supported sodium metal, regions of the chain where the helical sense reverses (switching from *P* to *M* screw sense) are prone to backbiting reactions that terminate chain growth. The authors succeeded in raising the proportion of longer chains in the product distribution by running the reaction in enantiomerically pure limonene, a relatively inexpensive and unreactive chiral liquid. This effect increased at higher reaction temperatures: At 90°C, the weight-average molecular weight, measured using size exclusion chromatography, more than doubled when the optically pure solvent was used in place of racemic limonene, presumably because of a reduced number of reversal sites. Investigation by optical absorption and circular dichroism spectroscopy supported a mechanism in which the chiral solvent stabilized a particular helical conformation of the growing polymer chain. — PDS

J. Am. Chem. Soc. **128**, 10.1021/ja064587e (2006).

ECOLOGY/EVOLUTION

Small-World Networks

Loss of habitat is a pervasive problem affecting species and ecological communities, yet our ability to predict the effects of habitat loss on the population sizes of the species is surprisingly limited; this can, in turn, be a hindrance to conservation planning. However, there is increasing correlative evidence that the structure of food webs might pro-

vide important clues to the patterns of population change, and Gotelli and Ellison confirm this with experimental evidence from invertebrate communities inhabiting *Sarracenia* pitcher plants. The experiments involved reducing the volume of water in the pitchers and removing the predators at the top of the food chain (which are often the

first casualty of habitat loss),

and then monitoring the changes in abundance of the remaining species. The observed patterns of population change most closely conformed to path analytical models that incorporated food web structure. Despite the small size and relative simplicity of the *Sarracenia* micro-ecosystem, the structure of its food web is similar



The pitcher plant.

to that of larger ecosystems. Hence, it is plausible that these models can be used to predict patterns of abundance in response to habitat loss at larger scales. — AMS

PLoS Biol. **4**, 10.1371/journal.pbio.0040324 (2006).

GEOPHYSICS

Westward Migration

The effects of Hurricane Katrina have been felt further afield seismically as well as politically. Gerstoft *et al.* detected seismic activity in Califor-

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nia corresponding to pressure and surface waves generated by pounding ocean waves in the Gulf of Mexico during the height of the storm, 28 to 29 August 2005. The seismologists used beam-forming techniques to back-project very low frequency seismic energy received at an array of stations in southern California. Body waves at double the ocean wave frequency (0.1 to 0.2 Hz) rattled deep through the earth from their source in shallow water east of New Orleans during the storm and for 9 hours after its landfall. Surface waves were also detected across the Gulf and tracked the ocean wave frequency and higher harmonics. The seismic surface waves mimicked the ocean wave pattern, with higher frequencies emanating from the eastern side and lower frequencies to the west of the eye. Thus, both surface and body seismic waves were generated in shallow water by breaking ocean waves from Katrina, but different physical mechanisms couple the water and ground motions that produce them. — JB

Geophys. Res. Lett. **33**, 10.1029/2006GL027270 (2006).

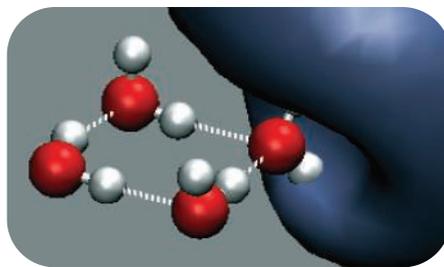
CHEMISTRY

Wet Quanta

Modern computers routinely allow efficient calculation of the geometries and electronic structures of neutral molecules using quantum-mechanical principles. However, charged species present a considerably greater challenge, and excess electrons are often treated by means of classical approximations. Herbert and Head-Gordon describe a method whereby the spatial distribution and detachment energy of an excess

electron bound to a tetrameric water cluster can be computed quantum-mechanically. These hydrated water clusters have been the subject of extensive recent experimental study in light of the fundamental questions they raise about bonding motifs, as well as their role as models for bulk hydrated electrons of interest in biological electron transfer and photodamage.

To render the method computationally tractable, the authors propagate the cluster atoms along a classical trajectory while applying



Calculated spatial distribution (blue) of an excess electron in a water cluster.

ab initio Møller-Plesset perturbation theory at each step to solve the electronic structure. The simulation results agree well with recent experimental measurements of vibrational and photoelectron spectra, and furthermore allow estimation of the cluster temperatures based on observed spectral widths. The authors note in closing that further advances in computing power should extend the applicability of the method to larger molecular clusters. — JSY

Proc. Natl. Acad. Sci. U.S.A. **103**, 10.1073/pnas.0603679103 (2006).



<< How Nickel Binding Regulates Transcription

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Bacteria, such as *Escherichia coli*, have enzymes that require nickel ions, and they express a nickel transporter to acquire the metal from the environment. To keep cellular concentrations of nickel relatively constant, the expression of the transporter is regulated by a repressor, NikR, which is itself a nickel sensor. NikR binds to the operator of the transporter gene and represses transcription only when it is in the nickel-bound form. Schreiter *et al* solved the crystal structures of the nickel-bound form of NikR from *E. coli* both alone and in a complex with a DNA fragment corresponding to the promoter of the nickel transporter gene. The protein has two DNA-binding domains that interact with sites in the palindromic operator on either side of a metal-binding domain. In other ligand-regulated transcription factors, activation is proposed to occur when a change in the spacing between the DNA-binding domains is altered in such a way that they interact more effectively with the promoter DNA. Comparison of the new structures with the previously reported structure of nickel-free protein indicates that this is not how NikR works. Rather, it appears to create a new interactive surface within the metal-binding domain that enhances the interaction of the protein with the promoter DNA helix. The results provide a detailed look at the precise molecular changes that underlie transcriptional control by a ligand-regulated transcription factor. — LBR

Proc. Natl. Acad. Sci. U.S.A. **103**, 13676 (2006).

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