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Department of Civil Engineering

Modeling a Rolling Wheel on Soil

Since their origin over three millennia ago, wheeled vehicles in transportation have become indisputably significant, with their presence ubiquitous all over the world. Volumes of empirical data based on carefully designed experiments and sophisticated theories have led to enormous improvements towards safe, comfortable, and easy operation of a variety of wheeled vehicles and machinery. Likewise, road engineering has advanced tremendously and better road surfaces are constantly being developed to accept increased vehicle speed and weight.

Beyond the realm of pavements, a particular area of continuous research interest is the interaction of a vehicle's rotating wheels and the unimproved, natural earth surface. In the 1960s this field of study acquired the name *Terramechanics*, as it deals with the mechanical behavior of the earth surface subjected to vehicle and machinery loads. In most cases the natural surface is soil, although vehicle movement over snow cover or ice also falls into this area.

In Terramechanics, empirically derived concepts thrive and they are rightly well-respected. There appear to be cases, however, where empiricism encounters great obstacles, an example being the operation of wheeled planetary

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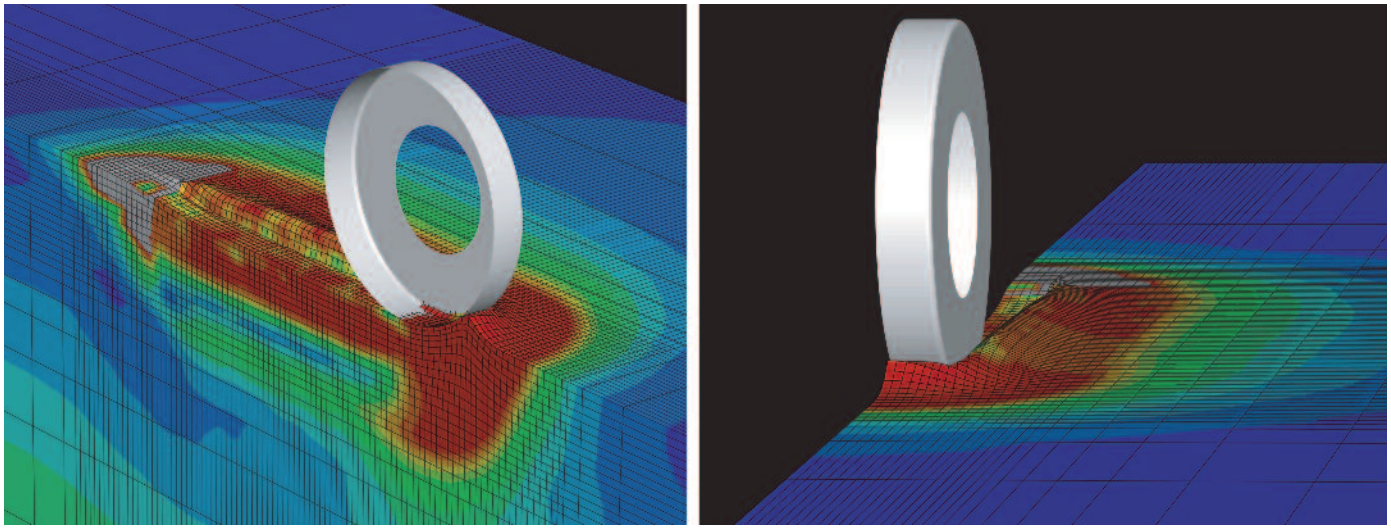

Figure 1. Deformed configuration at end of rolling wheel simulation. One half of the full problem is modeled by utilizing the plane of symmetry of the wheel midplane, and contours are of maximum shear stress.

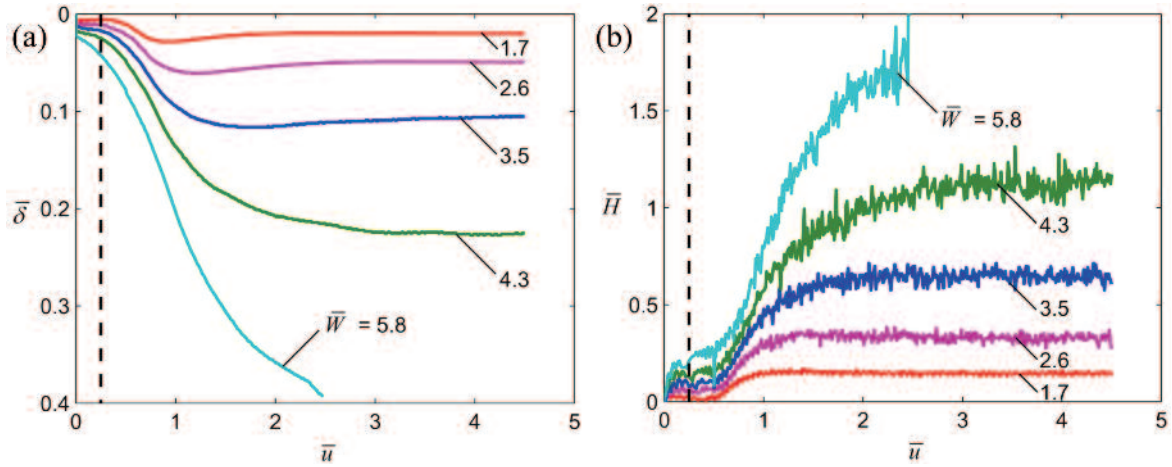

Figure 2. Normalized (a) wheel penetration and (b) horizontal force as functions of normalized rolling distance in clay-type material for varying applied weights.

rovers. Indeed, one of the Martian surveyors is no longer traveling because its wheels sank excessively in granular soil. A viable alternative to empiricism is analytical or numerical mechanics-based analysis of the interaction between the wheels and supporting soil or snow.

A narrow wheel rolling over permanently deforming soil belongs to a challenging class of problems involving three-dimensional geometry and physically non-linear phenomena. Analytical methods are difficult to formulate for such problems, making numerical simulation one of the only viable means for rigorous and accurate analysis. Continuum-based computations using the Finite Element Method (FEM) are a particularly powerful and effective tool for predicting the large, permanent deformations involved in soil-wheel interaction.

Using the finite element code ABAQUS/Explicit available at the Minnesota Supercomputing Institute, Professor Andrew Drescher, Department of Civil Engineering and MSI Associate Fellow, and Ph.D. student Jim Hambleton have performed extensive simulations to investigate how wheel-induced soil deformation is influenced by material type, layering, wheel geometry, loading, and interface friction at the soil-wheel interface. Elastic-plastic non-linear constitutive models were postulated to capture basic mechanical response of the soil, considering models representative of both clayey and sandy soil types. The Arbitrary Lagrangian-Eulerian (ALE) remeshing option was used to allow for accurate computations in the presence of large deformations, which are manifested as deep ruts, a front lip, and side berms formed during initial and steady rolling of the wheel (Figure 1).

The relationship between the rolling distance and the penetration of a narrow wheel subjected to various vertical forces (weight) is depicted in Figure 2a. The wheel is torque free (i.e., towed or pushed) and operates on clay-type material. In the figure, the following dimensionless variables are employed:

$$\overline{\delta} = \frac{\delta}{r}, \overline{b} = \frac{b}{r}, \overline{u} = \frac{u}{r}, \overline{W} = \frac{W}{kbr}, \overline{H} = \frac{H}{kbr}$$

where δ denotes wheel penetration, r is wheel radius, b is wheel width, u is translational displacement of the wheel, W is applied weight, H is the horizontal reaction force, and k is cohesion, or shear strength, of the soil. If the vertical load is not excessive, upon initial sinking the wheel typically undergoes small upward movement, eventually reaching a steady state of travel at a constant penetration. Also the corresponding horizontal force developing during rolling reaches a constant value (Figure 2b).

An important aspect of numerical simulation of the rolling process was discovered when attempting to model the problem as two-dimensional (plane strain). Plane-strain modeling has been widely used in numerous solid mechanics problems, and geomechanics problems in particular, because it greatly simplifies and speeds up computations. When modeling plane-strain rolling of a wheel over clay it became evident that no rut is formed behind the wheel, which in the steady state travels essentially at ground level. An increase in the weight of wheel only

produces an enlarged lip in front of the wheel (Figure 3). This phenomenon indicates that plane-strain analyses may not be capable of reproducing the actual three-dimensional features of the rolling process and may lead to physically erroneous conclusions.

In addition to numerical simulations, the authors have proposed a simplified, approximate analytic approach based on the fundamental solution of rigid punch indentation into a plastic half-space. With proper account for geometry changes during the indentation and rolling phases, the process can be modeled as a sequence of incipient plastic flow problems. This approximate approach agrees reasonably well with the more accurate numerical simulations and yields formulas that are amenable for usage in practice.

The numerical simulations and approximate analytic solutions also have been validated with results of small-scale experiments performed in the laboratory on clay and sand. Experimental techniques include the use of Particle Image Velocimetry (PIV), which allows for comparison between the real and predicted deformation fields at the wheel midplane. Satisfactory agreement between the theory and experiments has been demonstrated.

One novel application of the models described above originates from cooperation with the Minnesota Department of Transportation to evaluate the so-called "test rolling" procedure used for assessing the quality of subgrade compaction. Based on this work, the researchers have proposed using measurement of the permanent ruts left by wheels as a means for in situ evaluation of soil strength parameters. In essence, this is a non-linear inverse problem, and when resolved it provides a continuous log of strength properties over some distance. This feature of testing via a rolling wheel offers an attractive alternative to local strength measurements utilizing the variety of indenters and penetrometers presently dominating practice. Useful graphs have been constructed that relate the internal friction angle and cohesion, the two most important soil strength parameters, to steady-state wheel penetration.

Results of numerical and analytical analysis of wheel-soil interaction may also find application in assessing and preventing damage to land caused by off-road vehicles (ORVs). When used carelessly, ORVs such as ATVs, dirt bikes, and hauling trucks cause detrimental changes in deserts, forests, and tundra, thereby reducing the economic and societal value of the land. The main cause is the stripping of organic matter and vegetation, characterized by formation of permanent ruts created by rolling and spinning wheels (Figure 4). Vegetation provides strengthening (reinforcement) of the top layer of soil, and its disappearance exposes the soil to wind and water erosion. In open and arid regions, ruts channel water during spring runoffs and increase flow velocity and soil erosion. In forests, ruts expose tree roots, collect water, and make logging and recreational roads impassable. The negative impact of ORVs has been long recognized, and regulatory laws have been enacted or are being discussed. Expanding the research described above could contribute to a better understanding of the mechanics of rut formation, which ultimately would allow for formulation of

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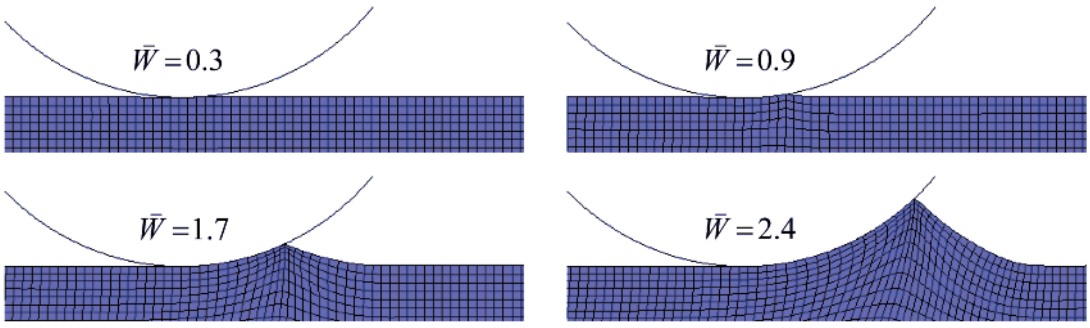

Figure 3. Deformed configuration in steady state from two-dimensional (plane-strain) simulation with various applied weights.

Figure 4. Region in the Wasatch-Cache National Forest (Utah) where negative impact of ORVs is evident (Photo courtesy of Dan Schroeder, Ogden Sierra Club).

improved guidelines on the design and use of ORVs.

The power of numerical simulations, approximate analytic methods, and small-scale experiments all point to new avenues of research in wheel-soil interaction, where applications range from terrestrial and extraterrestrial vehicle mobility to evaluation of field properties and land damage prevention. Additional details regarding this work can be found in a number of journal articles and conference proceedings, including:

- Hambleton, J.P., and Drescher, A. (2008a). Mechanistic approach for relating test roller penetration to mechanical properties of bases and subgrades. *Transportation Research Board 87th Annual Meeting Compendium of Papers*, Washington, D.C., USA, Jan. 13–17.
- Hambleton, J.P., and Drescher, A. (2008b). Soil damage models for off-road vehicles. *Proceedings of Geocongress 2008, Geosustainability and Geohazard Mitigation*, New Orleans, USA, Mar. 9–12, ASCE, Geotechnical Special Publication No. 178, 562-569.
- Hambleton, J.P., and Drescher, A. (2008c). Modeling wheel-induced rutting in soils: Indentation. *Journal of Terramechanics*, **45(6)**, 201–211.
- Hambleton, J.P., and Drescher, A. (2009a). Modeling wheel-induced rutting in soils: Rolling. *Journal of Terramechanics*, **46(2)**, 35–47.
- Hambleton, J.P., and Drescher, A. (2009b). On modeling a rolling wheel in the presence of plastic deformation as a three- or two-dimensional process. *International Journal of Mechanical Sciences*, **51(11-12)**, 84–-855.

Understanding and Predicting Properties of Nanostructures: Insights From Atomic-level Simulations

Tubes, rods, plates, shells, etc., are ubiquitous engineering structures, traditionally imagined as continuous objects. Their mechanical behavior is usually studied with the computational engineering tools of the continuum scale, based on the relations of macroscopic elasticity. These methods are computationally efficient, since they do not need to track every single nucleus. Thermodynamic quantities, such as temperature, are represented as fields. Behind this static elastic continuum is the effervescent world of mechanics—nanomechanics—where temperature represents the kinetic energy of the random motion of an order of 10^{23} microscopic entities. This discrete behavior shapes the experimentally verifiable constitutive laws of the continuum.

Nano-tubes, -wires, -coils, and -spheres are novel organizations of matter that became possible with recent advances in synthetic methods. For these structures, macroscopic mechanics breaks down and new mechanical behavior emerges. Understanding the new mechanics is important both fundamentally and practically because by capitalizing on the science emerging from the newly accessible size range, engineers can develop electromechanical devices, machines, and electronics on the nano scale. Professor Traian Dumitrica (Department of Mechanical Engineering and MSI Associate Fellow) and his research group and collaborators are using advanced computational microscopic methods to obtain the accurate nanomechanical response and understand the fascinating properties of nanostructures directly from the interatomic interactions and the quantum mechanics of the electrons. A few examples are discussed next.

Mechanical Properties of Carbon Nanotubes

Carbon nanotubes are long, narrow, hollow cylinders with walls just one atom thick. About 80,000 times smaller than a human hair, they are about 100 times stronger than steel at one-sixth the weight. By comparison, Kevlar—the fiber used in most bulletproof body armor—is about five times stronger than an equal weight of steel. Finding out what makes them break involves the study of molecular bonds, atomic dynamics, and complex quantum phenomena. There are hundreds of different kinds of nanotubes, sometimes with radically different

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Figure 1. Carbon nanotubes can break in a brittle or plastic way, according to microscopic simulations.

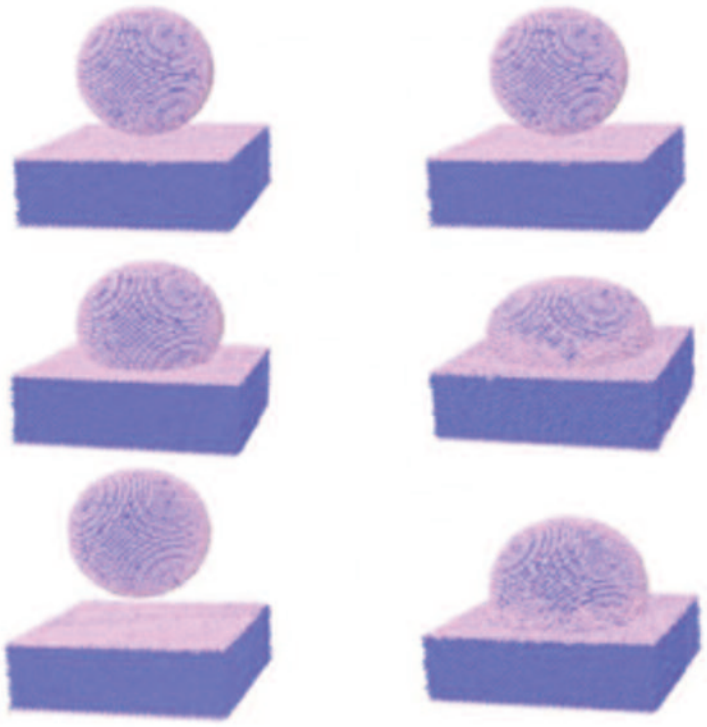

Figure 2. A nanoparticle containing some 30,000 silicon atoms and moving at 900 meters per second will bounce off a surface (left sequence), but at 2 km/s, it sticks (right sequence). The higher-speed impact causes two sequential changes in the crystalline structure.

properties. In spite of this complexity, computer simulations showed that nanotubes break in one of two ways: the bonds either snap in a brittle fashion or they stretch and deform (Figure 1). These mechanisms are each present at the same time and in one particular tensile test experiment, either type of break can occur. The researchers were able to obtain a pattern based on statistical probabilities of what is likely to occur in a range of conditions for the whole catalog of nanotube species. This result stands as an interesting example for the predictive power of simulations in materials science research.

Nanoparticle-surface collisions

In another project, researchers simulated the collision process of silicon nanoparticles with a substrate. In the everyday world, the harder you throw something like a basketball against the floor, the higher it will bounce. In the world of the very, very small, things bounce differently. Recently, colleagues of the Dumitrica group discovered that although silicon nanospheres are superhard, they stick to a substrate when colliding at 1–2 km/s. Molecular dynamics simulations (Figure 2) explain this puzzling result in a surprising way: although the contact force is relatively low by macroscopic standards, the impact pressure causes the high speed particle to change its crystalline structure and soak up so much energy that the particle can't bounce away. This understanding may help develop wear-resistant coatings created by many such high-speed impacts.

Manipulating the optical response of silicon quantum dots for energy applications

Silicon dots can have various sizes, shapes and core structures. The exhibited photoluminescence shows a tremendous potential for applications in the area of energy. However, an important challenge is adjusting the optical response by manipulating the electronic states around the last occupied, first empty levels. In crystals this is usually achieved by doping but this route proves to be difficult at the nanoscale. Until recently, the relationship between the intrinsic symmetry and the optical response of silicon quantum dots has been overlooked. Relying on the general concept of symmetry lowering, recent calculations indicate new effective routes to modulate the optical response of these tiny structures without affecting their stability. As in atoms, high symmetry in silicon dots brings electronic degeneracies and large level spacings, and enforces strict selection rules for the optical transitions between levels. Many transitions are forbidden. For instance, the energy spacing between last occupied, first empty levels is generally different from the first possible excitation. Of course no symmetry implies no degeneracy and all transitions would be allowed.

The question addressed by the team led by Professor Dumitrica was whether it is possible to alter the atom-like electronic levels of such dots without considering the unlikely endohedral doping. In atoms, splitting the degenerate energy levels is usually accomplished by breaking the symmetry with the help of an external magnetic field. In silicon dots, the researchers demonstrated via density-functional theory calculations that symmetry lowering and level splitting could be readily accomplished in new ways. For example, introducing a slight structural imperfection vis-à-vis the spherical shape (Figure 3) by applying mechanical squeezing and contaminating the surface with sodium atoms.

The continual development of nanotechnology will provide a greater range of highly symmetrical quantum dots. The uncovered connection between symmetry and electronic states makes these structures very exciting for both fundamental and applied research. In optoelectronics, symmetry lowering could become a useful strategy for manipulating the optical response.

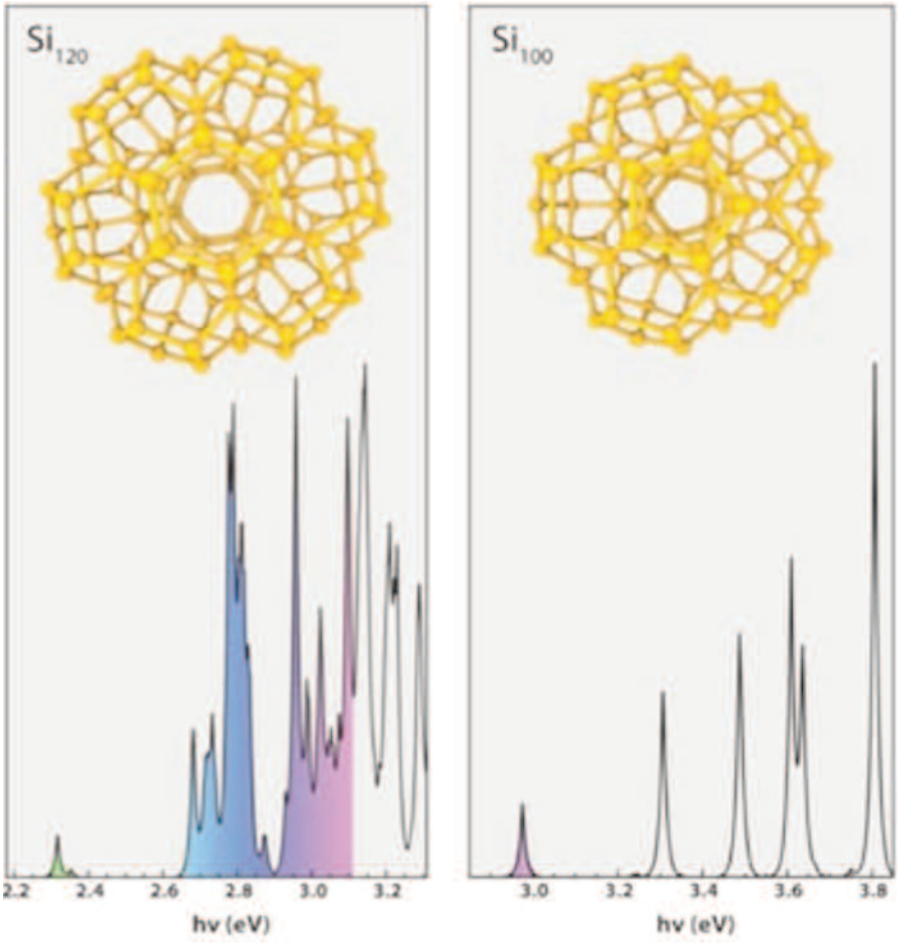

Figure 3. Two silicon dots that are similar in size (~2 nm), but slightly different in shape (left: oblate spheroid and right: spheroid) have different responses. Image credit: Yan Liang, University of Minnesota.

MSI at SC09

MSI attended SC09, the annual Supercomputing Conference, on November 16–20, 2009. The conference was held in Portland, Oregon. MSI staff and researchers gave presentations on current projects using MSI resources.

Above: Dr. Ben Lynch, Lead Application Software Developer and Computational Chemistry Consultant, gives a presentation.

Below: Dr. Shuxia Zhang, Scientific Computation Consultant, and Brian Ropers-Huilman, Director of Systems Administration and Technical Operations, try out a three-dimensional "dancing cow" demonstration.

photos on this page courtesy Amy Danielson, OVPR

Arlington HS BioSMART Program Visit

On March 17, 2010, a group of students and teachers from the BioSMART program at Arlington High School in St. Paul, Minnesota visited MSI to learn about using supercomputers in scientific research. Arlington is a magnet school with a focus in science, math, and technology. The BioSMART (Biology, Science, Math, Academic Rigor, and Technology) program introduces students to careers in biotech industries.

Above: Dr. H. Birali Runesha, MSI Director of Scientific Computing and Applications, talks with students preparing a video in the Scientific Development and Visualization Laboratory.

Right: Students investigate the interior of a computer.

Aerospace Engineering and Mechanics

2009/157
An Effective Interaction Potential Model for the Shape Memory Alloy AuCd
V.S. Guthikonda and **R.S. Elliott**

2010/3
A Three-level Cartesian Geometry Based Implementation of the DSMC Method
D. Gao, C. Zhang, and **T.E. Schwartzentruber**

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Parallel Implementation of the Direct Simulation Monte Carlo Method for Shared Memory Architectures
D. Gao and **T. Schwartzentruber**

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Thermodynamic Modeling of Martensitic Phase Transformations
V.S. Guthikonda and **R.S. Elliott**

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M. Tesfaye, S.S. Yang, J.F.S. Lamb, H.-J. G. Jung, **D.A. Samac**, **C.P. Vance**, **J.W. Gronwald**, and **K.A. VandenBosch**

Astronomy

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Narrow Angle Tail Radio Galaxies as ICM Interaction Probes
D.H. Porter, P.J. Mendygral, and **T.W. Jones**

2009/135
Testing Observational Techniques With 3D MHD Jets in Clusters
P.J. Mendygral, S.M. O'Neill, and **T.W. Jones**

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Long Tails on Thermonuclear X-ray Bursts From Neutron Stars: A Signature of Inward Heating?
J.J.M. in'tZand, L. Keek, A. Cumming, **A. Heger**, J. Homan, and M. Mendez

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C.C. Joggerst, S.E. Woosley, and **A. Heger**

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S.M. O'Neill and **T.W. Jones**

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Turbulence-induced Magnetic Fields and Structure of Cosmic Ray Modified Shocks
A. Beresnyak, **T.W. Jones**, and A. Lazarian

2009/186
Three-dimensional Magnetohydrodynamic Simulations of Buoyant Bubbles in Galaxy Clusters
S.M. O'Neill, D.S. De Young, and **T.W. Jones**

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First Experience of Compressible Gas Dynamics Simulation on the Los Alamos Roadrunner Machine
P.R. Woodward, J. Jayaraj, P.-H. Lin, and W. Dai

BICB, UMR

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Identification of Dynamical Hinge Points of the L1 Ligase Molecular Switch
G.M. Giambasu, T.-S. Lee, **C.P. Sosa**, M.P. Robertson, W.G. Scott, and **D.M. York**

Biochemistry, Molecular Biology, and Biophysics

2009/132 and CB 2009-55
Crystallization and Preliminary X-ray Diffraction of Chlorite Dismutase From Dechloromonas aromatica *RCB*
B.R. Goblirsch, B.R. Streit, J.L. DuBois, and **C.M. Wilmot**

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A Refinement Protocol to Determine Structure, Topology, and Depth of Insertion of Membrane Proteins Using Hybrid Solution and Solid-state NMR Restraints
L. Shi, N.J. Traaseth, R. Verardi, A. Cembran, **J. Gao**, and **G. Veglia**

2009/143 and CB 2009-63
The University of Minnesota Biocatalysis/Biodegradation Database: Improving Public Access
J. Gao, **L.B.M. Ellis**, and **L.P. Wackett**

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A Dynamic Range Compression and Three-dimensional Peptide Fractionation Analysis Platform Expands Proteome Coverage and the Diagnostic Potential of Whole Saliva
S. Bandhakavi, M. Stone, G. Onsongo, S.K. Van Riper, and **T. Griffin**

2009/177 and CB 2009-73
An Extended Structure of the APOBEC3G Catalytic Domain Suggests a Unique Holoenzyme Model
E. Harjes, P.J. Gross, K.-M. Chen, Y. Lu, K. Shindo, R. Nowarski, J.D. Gross, M. Kotler, **R.S. Harris**, and **H. Matsuo**

Names of Supercomputing Institute principal investigators appear in bold type. This list contains reports entered into the reports database during Dec 2009–Mar 2010.

2009/187 and CB 2009-80
Reconstruction of Escherichia coli *Transcriptional Regulatory Networks via Regulon-based Associations*
H. Zare, D. Sangurdekar, P. Srivastava, M. Kaveh, and **A. Khodursky**

2009/188 and CB 2009-81
In Vivo *and* In Vitro *Patterns of the Activity of Simocyclinone D8, an Angucyclinone Antibiotic From* Streptomyces antibioticus
L.M. Oppegard, B.L. Hamann, K.R. Streck, K.C. Ellis, H.-P. Fiedler, **A.B. Khodursky**, and H. Hiasa

2009/189 and CB 2009-82
Improved Detection of Differentially Expressed Genes Through Incorporation of Gene Locations
G. Xiao, C. Reilly, and **A.B. Khodursky**

2009/250 and CB 2009-125
Ubiquitin-binding Domains—From Structures to Functions
I. Dikic, S. Wakatsuki, and **K.J. Walters**

2009/251 and CB 2009-126
Prokaryotic Ubiquitin-like Protein Pup Is Intrinsically Disordered
X. Chen, W.C. Solomon, Y. Kang, F. Cerda-Maira, K.H. Darwin, and **K.J. Walters**

2009/252 and CB 2009-127
Structure of the S5a:K48-Linked Diubiquitin Complex and Its Interactions With Rpn13
N. Zhang, Q. Wang, A. Ehlinger, L. Randles, J.W. Lary, Y. Kang, A. Haririnia, A.J. Storaska, J.L. Cole, D. Fushman, and **K.J. Walters**

2009/253 and CB 2009-128
Insights Into How Protein Dynamics Affects Arylamine N-acetyltransferase Catalysis
N. Zhang and **K.J. Walters**

2009/291 and CB 2009-149
Dual Mechanisms of sHA 14-1 in Inducing Cell Death Through Endoplasmic Reticulum and Mitochondria
D. Hermanson, S.N. Addo, A.A. Bajer, J.S. Marchant, S.G.K. Das, B. Srinivasan, F. Al-Mousa, F. Michelangeli, **D.D. Thomas**, T.W. LeBien, and C. Xing

Biology, UMD

2009/124 and CB 2009-48
Uncovering the Arabidopsis thaliana *Nectary Transcriptome: Investigation of Differential Gene Expression in Floral Nectariferous Tissues*
B.W. Kram, W.W. Xu, and **C.J. Carter**

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T. Netoff, Y. Park, and K. Parhi

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R. Raghupathy and **V.H. Barocas**

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Inhibiting Lateral Domain Formation in Lipid Bilayers: Simulations of Alternative Steroid Headgroup Chemistries
J.D. Perlmutter and **J.N. Sachs**

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Y. Chen and **S. Sarkanen**

Center for Drug Design

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D. Lu, **Y.Y. Sham**, and R. Vince

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K. Umemoto, **R.M. Wentzcovitch**, S. Saito, and T. Miyake

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K. Umemoto, **R.M. Wentzcovitch**, S. de Gironcoli, and S. Baroni

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C.R.S. da Silva, P.R.C. da Silveira, B. Karki, and **R.M. Wentzcovitch**

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A Boundary Element Method/Brownian Dynamics Approach for Simulating DNA Electrophoresis in Electrically Insulating Microfabricated Devices
J. Cho, M. Kenward, and **K.D. Dorfman**

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H. Hsu, K. Umemoto, P. Blaha, and **R.M. Wentzcovitch**

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S.A. Roberts and **S. Kumar**

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Extended DFT + U + V Method With On-site and Inter-site Electronic Interactions
V. Leiria Campo, Jr. and **M. Cococcioni**

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Mining Transcriptome Data for Function-Trait Relationship of Hyper Productivity of Recombinant Antibody
S. Charaniya, **G. Karypis**, and **W.-S. Hu**

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Structure-Kinetic Relationship Analysis of the Therapeutic Complement Inhibitor Compstatin
P. Magotti, D. Ricklin, H. Qu, Y.-Q. Wu, **Y.N. Kaznessis**, and J.D. Lambris

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Path-Integral Method for Predicting Relative Binding Affinities of Protein-Ligand Complexes
C. Mulakala and **Y.N. Kaznessis**

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Poisson-Nernst-Planck Models of Nonequilibrium Ion Electrodiffusion Through a Protegrin Transmembrane Pore
D.S. Bolintineanu, A. Sayyed-Ahmad, H.T. Davis, and **Y.N. Kaznessis**

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Determining the Orientation of Protegrin-1 in DLPC Bilayers Using an Implicit Solvent-Membrane Model
A. Sayyed-Ahmad and **Y.N. Kaznessis**

2009/259 and CB 2009-134
Forward Engineering of Synthetic Biological AND Gates
K.I. Ramalingam, J.R. Tomshine, J.A. Maynard, and **Y.N. Kaznessis**

2009/260 and CB 2009-135
Computational Methods in Synthetic Biology
Y.N. Kaznessis

2009/261 and CB 2009-136
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A. Sayyed-Ahmad, H. Khandelia, and **Y.N. Kaznessis**

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K. Umemoto and **R.M. Wentzcovitch**

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J. Schmidt, J. VandeVondele, I.-F.W. Kuo, D. Sebastiani, **J.I. Siepmann**, J. Hutter, and C.J. Mundy

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Monte Carlo Simulations of Binary Mixtures of Nitrotoluene Isomers With n*-Decane*
K.A. Maerzke and **J.I. Siepmann**

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Total Synthesis and Evaluation of C26-Hydroxyepothilone D Derivatives for Photoaffinity Labeling of β-Tubulin
E.A. Reiff, S.K. Nair, J.T. Henri, J.F. Greiner, B.S. Reddy, R. Chakrasali, S.A. David, T.-L. Chiu, **E.A. Amin**, R.H. Himes, D.G. Vander Velde, and **G.I. Georg**

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