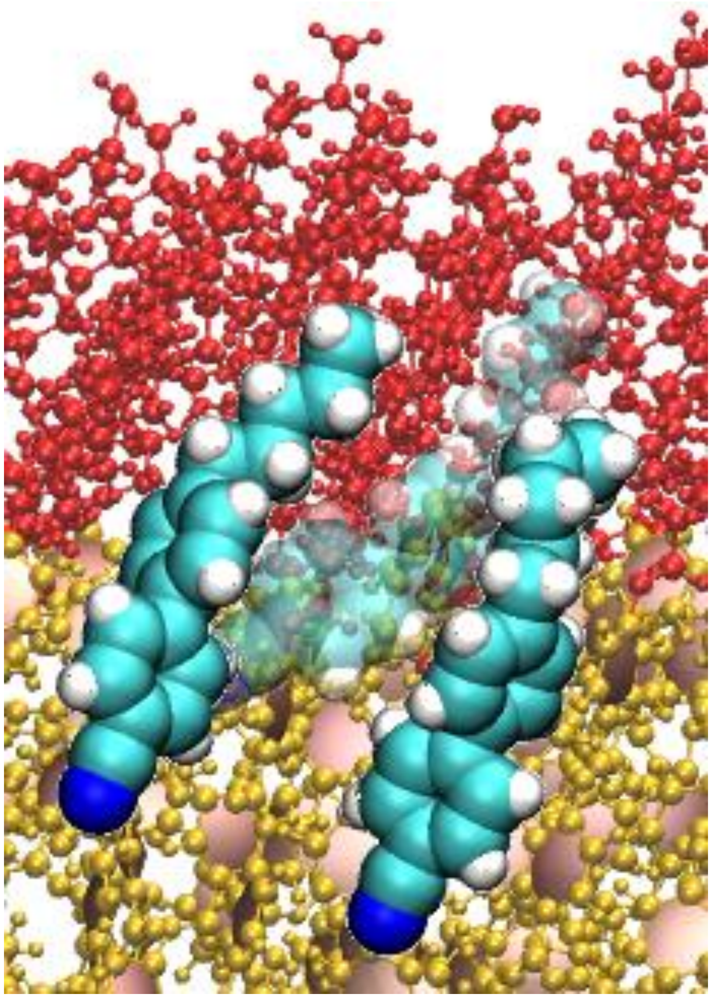


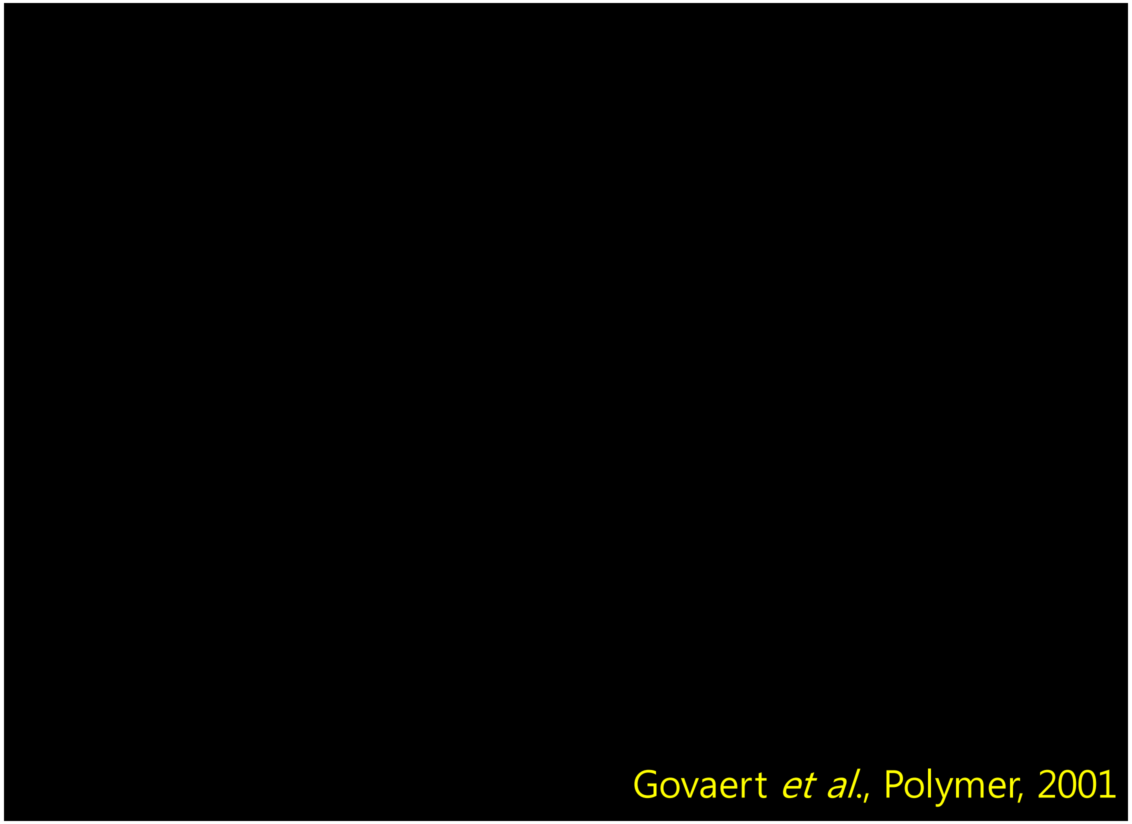
Molecular simulations research using OSC resources

Daniel Lacks
Department of Chemical Engineering
Case Western Reserve University

CASE SCHOOL OF ENGINEERING
CASE WESTERN RESERVE UNIVERSITY

How deformation enhances mobility in a polymer glass

Student:
Greg Chung

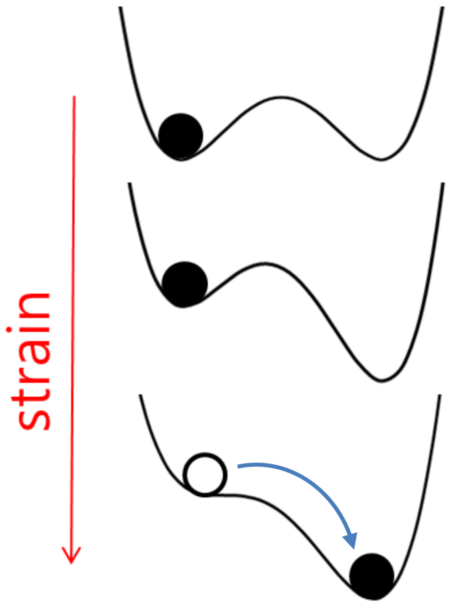


Govaert *et al.*, Polymer, 2001

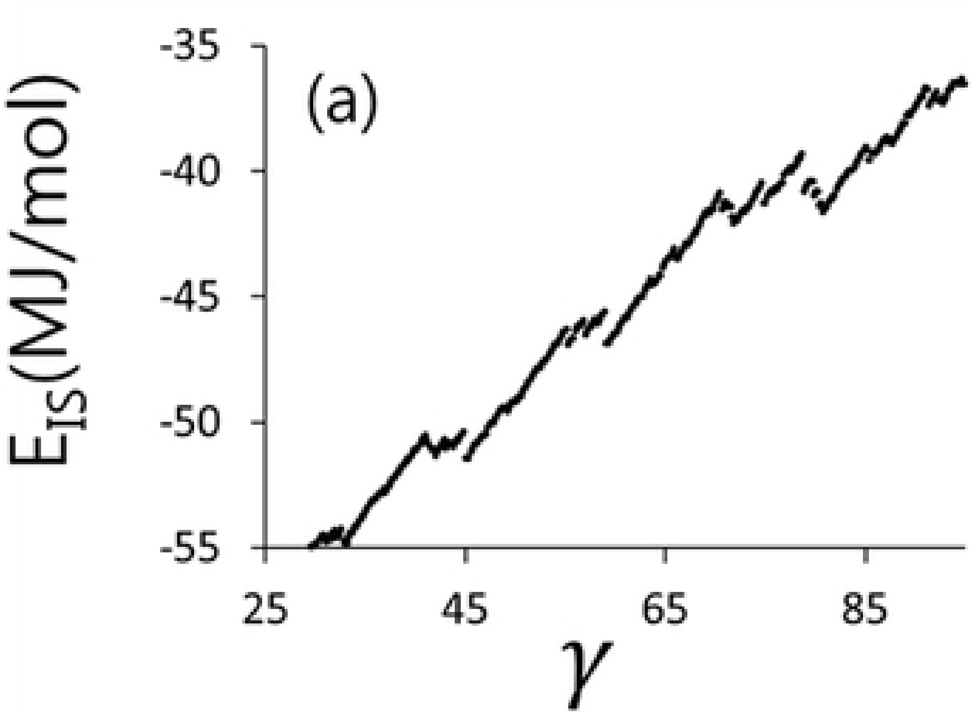
DMR-0705191

How deformation enhances mobility in a polymer glass

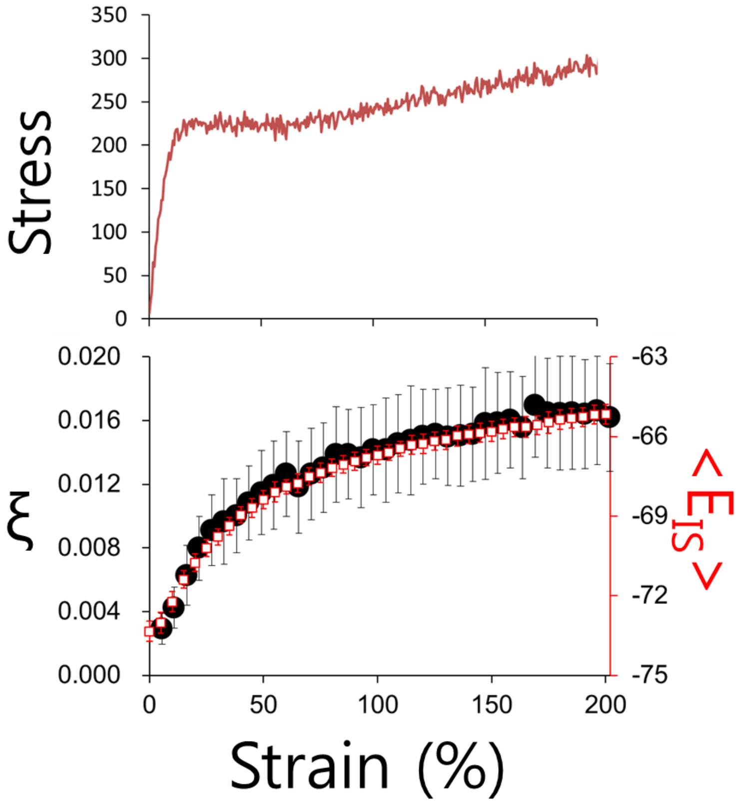
How deformation enhances mobility in a polymer glass

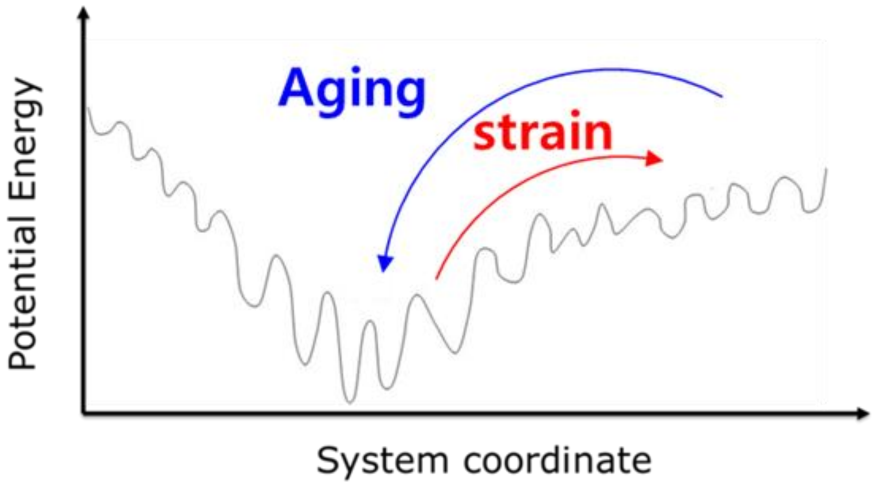


‘fold-catastrophe’



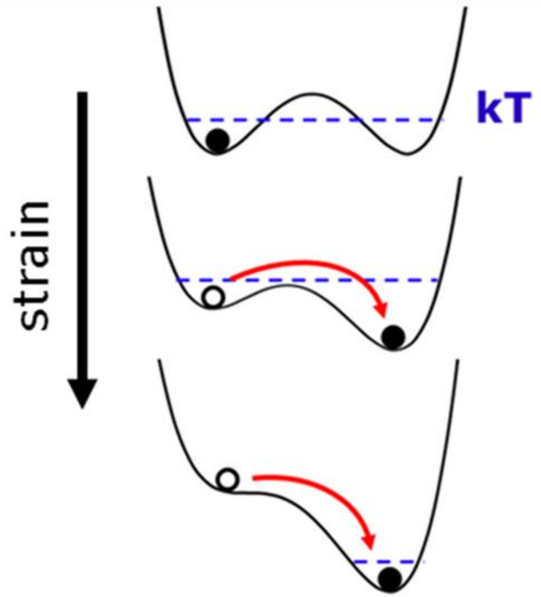
How deformation enhances mobility in a polymer glass



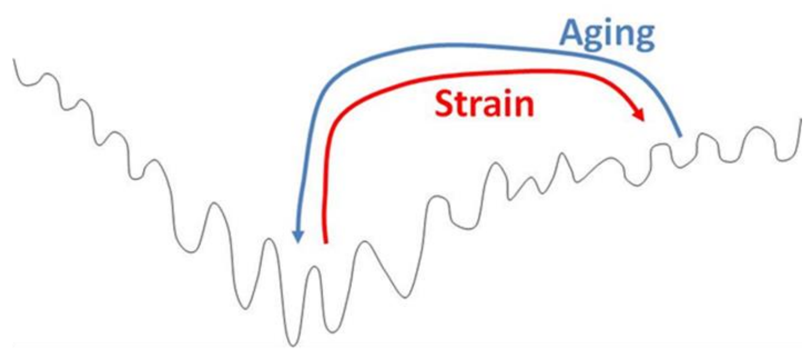


How deformation enhances mobility in a polymer glass

Reason 1
Strain reduces barriers



Reason 2
Strain moves system to regions of PEL with lower barriers



Chung, Y.G.; Lacks, D.J., Macromolecules, **45,** 10 (2012)

How deformation enhances mobility in a polymer glass

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November 06, 2013

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Returning Materials to a Youthful Form

NSF Award: Molecular Simulation of Disordered Materials under Stress (Case Western Reserve University)

State: Ohio

Congressional Districts: Ohio District 11

Research Areas: Chemistry & Materials

It is not uncommon to snap and break a plastic knob in an older car. The properties of plastics change slowly over time. Plastics can become brittle as the long molecules--the fundamental building blocks of plastics and polymeric materials more generally--degrade. Increasing the temperature of the material until it becomes molten and cooling it back down until it returns to a solid, can reverse the aging process. But can a mechanical deformation do the same thing?

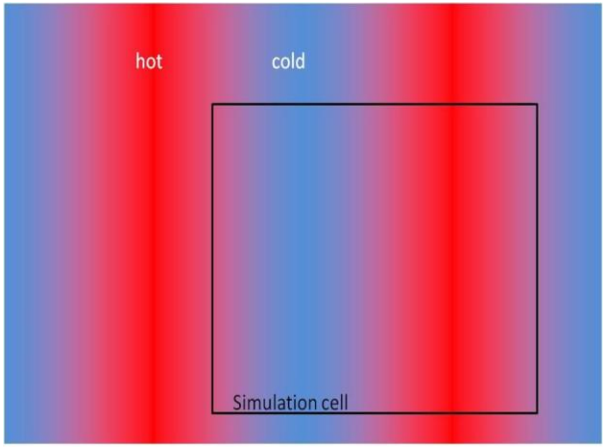
To answer this question, researcher Dan Lacks and student Greg Chung used a computer to simulate polystyrene molecules under shape-altering stress. Polystyrene appears in many applications including plastic drinking glasses and eating utensils. Lacks and Chung found that mechanical deformation can lead to macroscopic properties more like those of the plastic in its youth. But examination at the microscopic level shows that in contrast to the age reversing effects of temperature cycling, the mechanically rejuvenated material differs in a fundamental way--it is in a state that cannot be achieved by changing temperature alone. The insight gained

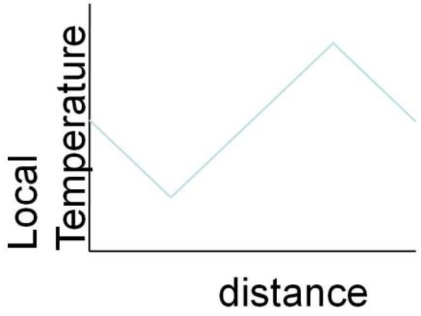
Image

Isotope fractionation in geological systems

Collaboration with experimentalists:
Chip Lesher (UC Davis)
Craig Lundstrom (U. Illinois – Urbana)
Jim Van Orman (CWRU)

Postdoc:
Gaurav Goel (CWRU)





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Isotope fractionation in geological systems

Isotope fractionation in geological systems

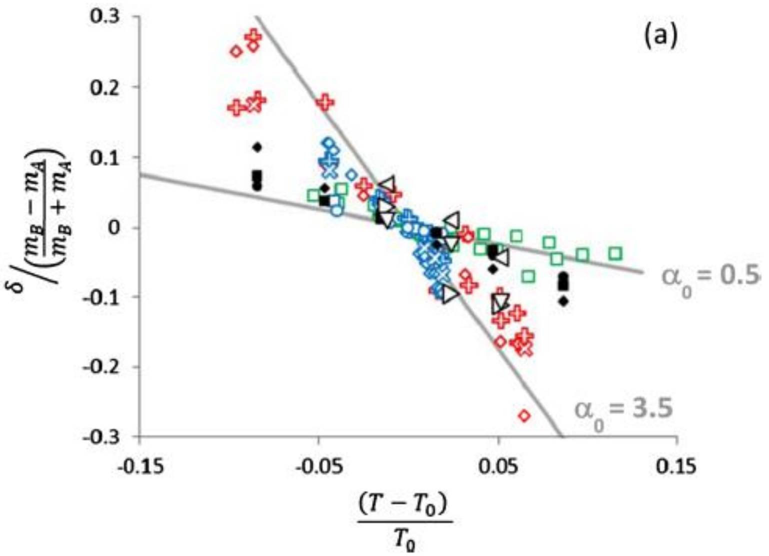
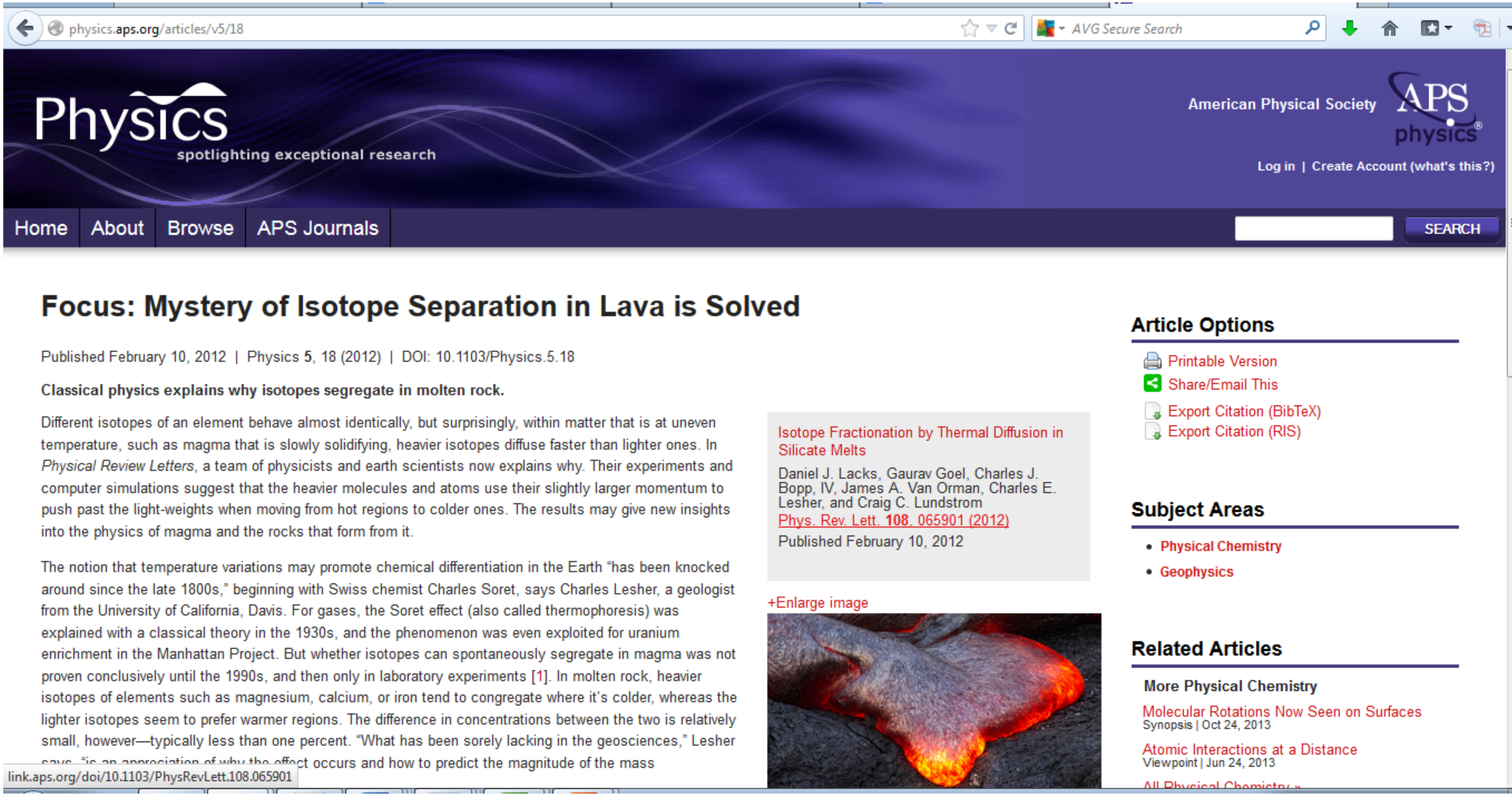


FIG. 2 (color online). Scaled presentation of experimental and MD results for isotope fractionation. Key: Open symbols are experimental results, filled symbols are MD results. ○ = Si; □ = O; ◇ = Mg; + = Fe; × = Ca; ▷ = Sr; ▽ = Hf; ◁ = U. (red) Huang *et al.*, [4] (blue) Richter *et al.*, [2,3] (green) Kyser *et al.*, [1], (black) new results.

Lacks, Goel, Bopp, Van Orman, Lesher, Lundstrom, *Phys. Rev. Lett.* **108**, 065901 (2012).

Isotope fractionation in geological systems



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Focus: Mystery of Isotope Separation in Lava is Solved

Published February 10, 2012 | Physics **5**, 18 (2012) | DOI: 10.1103/Physics.5.18

Classical physics explains why isotopes segregate in molten rock.

Different isotopes of an element behave almost identically, but surprisingly, within matter that is at uneven temperature, such as magma that is slowly solidifying, heavier isotopes diffuse faster than lighter ones. In *Physical Review Letters*, a team of physicists and earth scientists now explains why. Their experiments and computer simulations suggest that the heavier molecules and atoms use their slightly larger momentum to push past the light-weights when moving from hot regions to colder ones. The results may give new insights into the physics of magma and the rocks that form from it.

The notion that temperature variations may promote chemical differentiation in the Earth "has been knocked around since the late 1800s," beginning with Swiss chemist Charles Soret, says Charles Lesher, a geologist from the University of California, Davis. For gases, the Soret effect (also called thermophoresis) was explained with a classical theory in the 1930s, and the phenomenon was even exploited for uranium enrichment in the Manhattan Project. But whether isotopes can spontaneously segregate in magma was not proven conclusively until the 1990s, and then only in laboratory experiments [1]. In molten rock, heavier isotopes of elements such as magnesium, calcium, or iron tend to congregate where it's colder, whereas the lighter isotopes seem to prefer warmer regions. The difference in concentrations between the two is relatively small, however—typically less than one percent. "What has been sorely lacking in the geosciences," Lesher says, "is an appreciation of why the effect occurs and how to predict the magnitude of the mass

link.aps.org/doi/10.1103/PhysRevLett.108.065901

Isotope Fractionation by Thermal Diffusion in Silicate Melts

Daniel J. Lacks, Gaurav Goel, Charles J. Bopp, IV, James A. Van Orman, Charles E. Lesher, and Craig C. Lundstrom

Phys. Rev. Lett. **108**, 065901 (2012)

Published February 10, 2012

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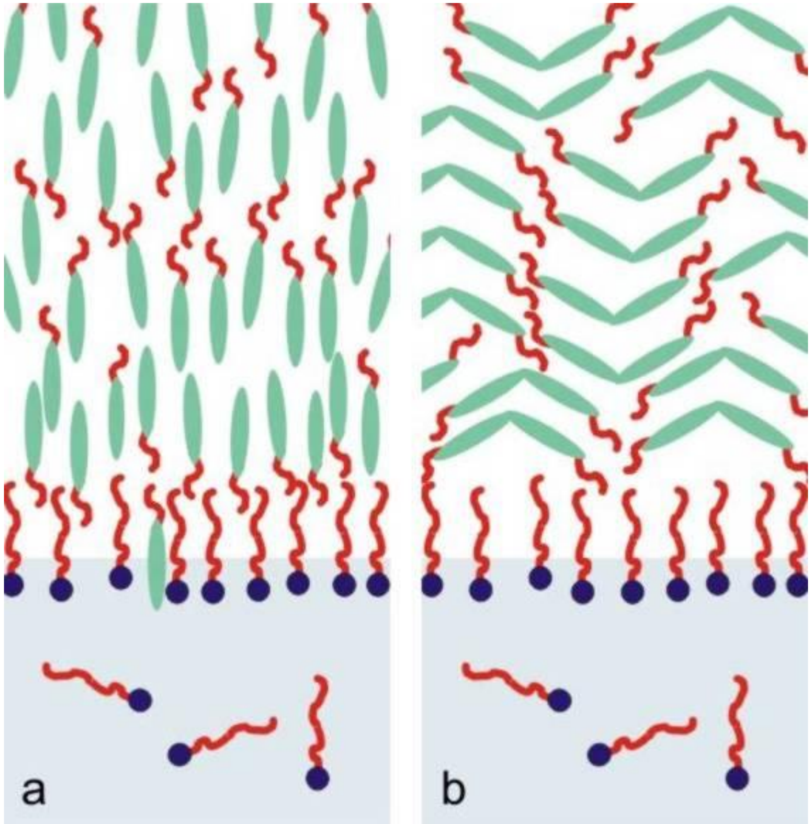
Self-assembly of bent-core liquid crystals at liquid surfaces

Collaboration with experimentalists at Kent State:
Elizabeth Mann (Physics)
Tony Jakli (Liquid Crystal Inst.)

Students:
Tim Smith (CWRU)
Wilder Iglesias (Kent)
Piotr Popov (Kent)



DMR-0906852

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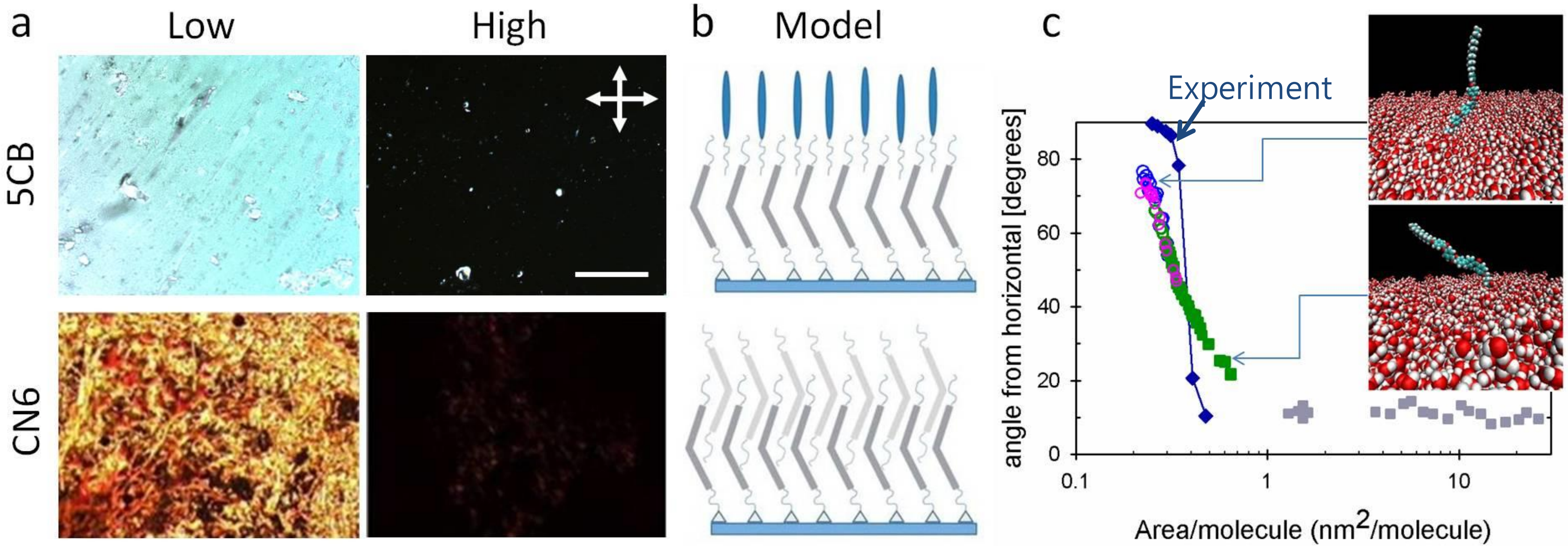
Self-assembly of bent-core liquid crystals at liquid surfaces

Self-assembly of bent-core liquid crystals at liquid surfaces



Iglesias, Smith, Basnet , Stefanovic, Tschierske, Lacks, Jákli, Mann, *Soft Matter* **7**, 9043 (2011)

Triboelectric charging

Collaboration with experimentalist:
Mohan Sankaran (CWRU)

Students/Postdocs:
Xiaozhou Shen (theory)
Andrew Wang
Mihai Bilici
Mamadou Sow
Joe Toth
Ross Widenor
Richard Pham

CBET-1235908
DMR-1206380

PARTICLE CLOUDS

Frictile attraction

Clouds of uncharged particles such as sand or volcanic ash become charged by some undetermined mechanism. Experiments now show that nearby electric fields could be responsible.

Daniel J. Lacks

Have you ever received a shock on touching a door-knob after shuffling across a carpet? The culprit, known as triboelectric charging, is also responsible for phenomena as innocuous as a rubbed balloon that makes your hair stand on end, or as dramatic as a lightning strike. Despite being familiar to every child, fundamental understanding of triboelectric charging is so poor that even the most basic questions are still being debated, such as whether the transferred charge species are electrons or ions[1,2]. Scientific progress in this field is difficult because triboelectric charging is a non-equilibrium process (separated surfaces are neutral at equilibrium) that involves changes in electron states and occurs at a level of one electron per 100,000 surface atoms (physical and/or chemical defects at this low level probably control the behaviour). As reported in *Nature Physics*, Thomas Pähtz *et al.*[3] take a key step towards understanding triboelectric charging by showing that external electric fields can play a role in the charging process.

An important consequence of triboelectric charging, in industry and the natural world, involves particle clouds. These clouds can be formed by granular systems consisting of particles that are small enough to be easily dispersed into the atmosphere (less than roughly 1 mm). In arid environments, soil is kicked up by wind, or by the movement of people, equipment and animals, to create dust clouds. Volcanic eruptions and fires produce clouds of ash by a more violent process. In industrial operations, the transfer of powder materials can result in the formation of particle clouds. It is generally accepted that the particles in these clouds become electrostatically charged, presumably by collisions with one another. As the particles settle from the cloud, they often adhere strongly to objects owing to the electrostatic charge. This charge-enhanced

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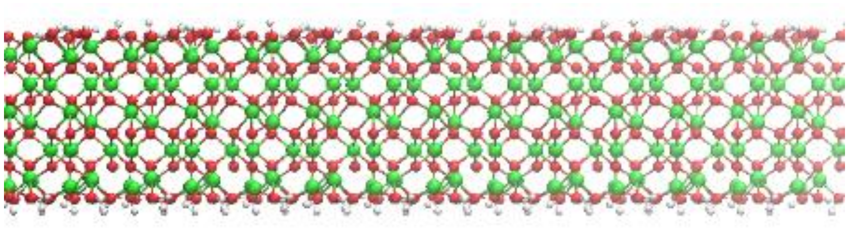
Triboelectric charging

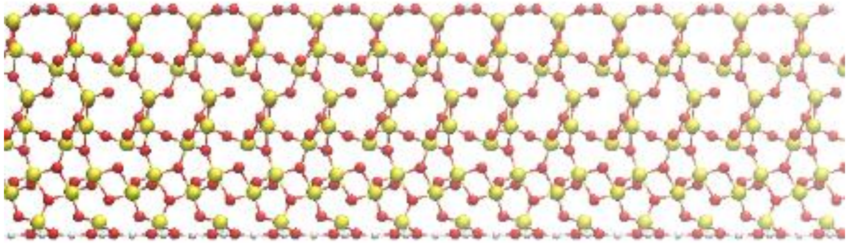
Triboelectric charging

Our plan: Focus on a simple system that can be addressed rigorously both experimentally and theoretically.

Defined crystallographic faces of SiO_2 quartz and Al_2O_3 sapphire

Theory – use electronic structure simulations (SIESTA). Will include water at surfaces to allow for ion mechanisms.

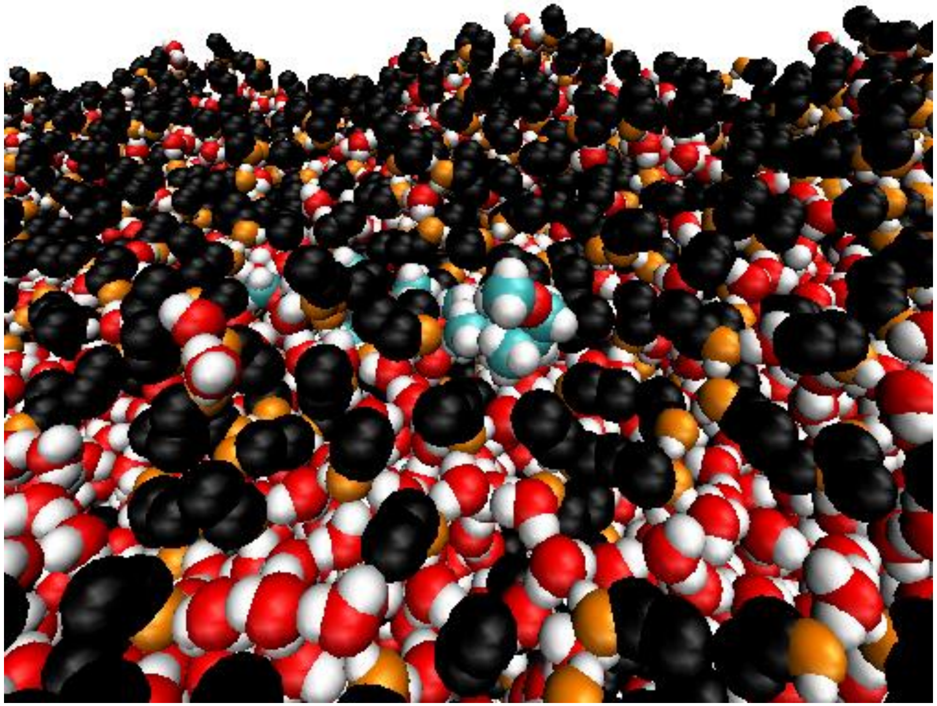




Surfactants in mixed solvent systems

Collaboration with experimentalist:
We’re doing the experiments ou
rselves!

Students:
Guy Mongelli
Raven Alford



CBET-1159327

Thank you OSC!!

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