CHEM MAJOR NEWS

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Student Affiliates at the University of Pittsburgh

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THE WELCOME BACK EDITION

Welcome back, y'all! It's that time of year again. Soon, autumn will officially be here and with it will come shorter days and cooler temperatures. Most importantly (I'm being facetious), any day now, we will begin to witness an annual phenomenon unique to our 21st century western world. We will soon experience PUMPKIN EVERYTHING. At the root of this yearly pumpkin frenzy is a certain pumpkin spice latte made by a certain coffee company, which shall not be named here, though I will say that its name rhymes with "aw shucks." And if we're lucky, this particular coffee company will keep plenty of pumpkin spice latte on hand throughout the season; after all, I'd hate to see a repeat of the great pumpkin spice latte shortage of 2012. It was so traumatic that diehard fans of this signature drink did the only thing they could do in such a situation…they furiously expressed their outrage via 140 character status updates.

All joking aside, the beginning of the fall semester is a great time to sit down and take a good look at your college career thus far and to remind yourself of where you'd like to go from here. If you're a freshman, you haven't experienced much of college yet and during these first few months, you will be bombarded with options. For example, you might be tempted to get involved in all sorts of extracurricular activities, school sanctioned or otherwise. Whatever the case may be, I strongly encourage you to ask yourself where you want to be in one year, two years, three years, and so forth, and to be honest with yourself about how much you can handle. Then, make a plan and stick to it because college is going to be quite unlike any challenge most of you have ever encountered.

The same goes for sophomores and juniors. You now have some experience under your belt and have a better idea of what it will take to succeed at this level. Perhaps you took some challenging classes and did not do as well as you would have liked. Maybe you took on too many extracurricular responsibilities or spent too much time fooling around and not enough time focusing on your coursework. If you haven't already done so, this is the perfect time to reevaluate your priorities and plans and to figure out what you need to do to be successful. I'm speaking from experience and I can tell you that it's not too late to turn it around!

As for you seniors, I urge you to finish strong. Don't let off the gas now! I too am in my final year of being an undergraduate and I'm looking forward to all of the great things that will come with graduating; however, it's crucial that we remember that what we do in this final year still counts, still goes on record. Life continues after graduation but most of us have just one chance to finish strong and preserve all of the hard work we've put in over the last two or three years. So let's make the most of this brand new semester, this fresh start!

Last but certainly not least, if you enjoy chemistry (who doesn't?) and desire greater involvement in community outreach, consider becoming a member of the University of Pittsburgh chapter of the American Chemical Society (ACS). More information about the rewarding opportunities provided through membership in ACS can be found in the main office of Chevron Science Center. Once again, welcome back to Pitt and I wish you success as you press on into another semester!

Slàinte Mhath!
Trevor Hyland, *Newsletter Co-Editor*

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Quantum Computers and Chemistry

by: James Toye

Quantum computing is a term that we see pop up more and more in news media - the technology of the future, making research bigger, better, and faster. But what is quantum computing, can it help researchers in chemistry, and if so, how? Over the next few paragraphs we will take a look into this budding technology and at some of the more recent discussion of its application in our field.

Traditional computers store pieces of data in units called bits. Any given bit has two states, 1 or 0, on or off. While computing technology has made huge leaps in both ability to store and access information, it remains very difficult to run simulations of quantum systems on these machines. As the system of interest grows, the amount of processing power and space needed on the computer grows exponentially. This growth makes simulating even small systems difficult.

On the other hand, quantum computers store data in units called qubits. These also have the same 1 and 0 states, but these states can also exist in a superposition, where the qubit exhibits qualities of both. Varieties of these superpositions exist, allowing for exponentially more storage states. Research from late last decade indicates that this alternate method of storing and representing data can reduce the drain on the computing system to a polynomial rate (n * x versus n^x). This change in operating cost would allow quantum machines of one hundred qubits to perform as well as traditional computers.

By early this decade, quantum computing had already been applied to research in chemistry. The energy of an H2 molecule was calculated with an iterative phase estimation algorithm, where a number of measurements are made, then quantified as a 20 bit number, which agreed with a simulation performed on a traditional computer. This quantum calculation only involved two qubits, and demonstrated that for larger systems the computing requirements would not scale exponentially, making larger simulations more likely in the future.

As a counterpoint, in 2014 research was published indicating that while the amount of storage resources needed to run these simulations may be less for larger molecules, larger amounts of other resources may be required to solve the algorithms needed to make use of the data, or more efficient algorithms will need to be developed in order to make use of this blossoming technology. Though this research indicates that it may still be some time before quantum computing becomes a mainstay of chemical research, it does appear to be something worth keeping an eye on. Large leaps have already been made in the application of quantum computing, and as the field continues to develop, this author has no doubt that exciting things will come.

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A Few Truths About Fracking

Keith Kennedy, Monthly Contributor

Fracking has been a hot topic in the news throughout the last few years. I'm sure that we all know the basics about fracking. Most know that fracking is a method of extracting natural gas from natural gas rich ground. Most will also probably know that the safety of this type of natural gas drilling is under constant debate. In order to form a more informed opinion on the matter let's take a look a few hard facts.

First, lets talk about how the fracking process works. Fracking starts with drilling. A well is drilled deep into the earth's crust, below ground water, into the natural gas or oil containing shale. The initial well is drilled straight downward. This well is encased in steel piping and concrete. Once the well is deep enough to meet the gas rich shale, horizontal drilling along the shale begins. After encasing the newly drilled well in steel, a perforating tool is used to crack or fracture the surrounding shale. Next, extracting fluid consisting of mostly water and sand is pumped into these cracks. When the fluid is pumped back out, the sand is able to keep the fractures open, allowing for the natural gas to flow intom and out of the well.

The extraction fluid used in 99.5% water and sand, but what is in that other 0.5%? Many drilling companies are conspicuously vague about the last 0.5% of the fluid, but perhaps this is just to protect their intellectual property from those who might steal it. When I looked into this further I found that this last 0.5% of fluid is composed of a multitude of chemicals. Some of the chemical such as Citric Acid (vitamin C) and Sodium Chloride (table salt) are harmless. Some of the other components seemed more menacing. For example, Triethanolamine Zirconate is listed as one of these chemicals. Triethanolamine Zirconate is also listed as a carcinogen. Methanol and other flammable substances are also among the 0.5%.

There is no harm in the use of these potentially dangerous chemicals as long as they are properly disposed of. Most drilling companies insist that the drilling is safe and no harmful chemicals from the extraction solution ever reach the surface. In many cases, however, the inhabitance of the areas surrounding fracking wells report major changes in the quality of their drinking water.

USA Today reported that Pennsylvania, Ohio, and West Virginia have all reported drinking water contamination as a result of natural gas drilling. Testing showed that a high concentration of heavy metals, as well as very high chloride concentration were found in the contaminated water. It is true that most drilling sites do not seem to affect the water quality, but those that are affected report some startling information. Those who ingest the contaminated water report feeling ill and fear long-term health effects. In one case, someone reported that the water pumped from their well became flammable as a result of fracking nearby.

So the real question is, is fracking worth it? It is no secret that fracking creates jobs and make drilling companies a whole lot of money, but at what cost?

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http://www.USAtoday.com
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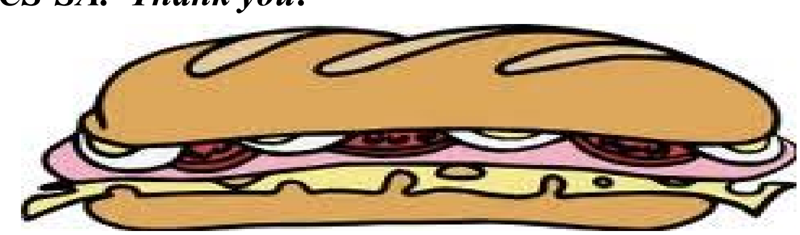
The ACS-SA will be selling hoagies every Tuesday at lunchtime in the lobby of Chevron Science Center. This year they will be from Uncle Sam's! Details are coming soon...Please support our ACS-SA. Thank you!



Green Chemistry

by: Raissa Berry, Green Chemistry Contributor, 2013-2014

My name is Raissa Berry, I am a junior neuroscience major with hopes of attending medical school. Last spring, I became an ACS member and immediately felt like I had been a member forever. Everyone was so friendly and welcoming, making me want to get more involved in the various events and volunteering opportunities ACS offers. This year, I will be writing the Green Chemistry column for the ACS newsletter. This first article will examine the basics, followed by articles regarding real-world use and progress of Green Chemistry. Defined as the proposal, creation and use of chemical artifacts and procedures to abolish or diminish the creation of residues harmful to our health and the environment,1 there are twelve principles of Green Chemistry:

The Twelve Principles of Green Chemistry

1. **Prevention –** It is better to prevent waste than to treat or clean up waste after it has been created.

2. **Atom Economy –** Synthetic methods should be designed to maximize the incorporation of all materials used in the process into the final product.

3. **Less Hazardous Chemical Syntheses –** Wherever practicable, synthetic methods should be designed to use and generate substances that possess little or no toxicity to human health and the environment.

4. **Designing Safer Chemicals –** Chemical products should be designed to affect their desired function while minimizing their toxicity.

5. **Safer Solvent and Auxiliaries –** The use of auxiliary substances (e.g., solvents, separation agents, etc.) should be made unnecessary wherever possible and innocuous when used.

6. **Design for Energy Efficiency –** Energy requirements of chemical processes should be recognized for their environmental and economic impacts and should be minimized. If possible, synthetic methods should be conducted at ambient temperature and pressure.

7. **Use of Renewable Feedstocks –** A raw material or feedstock should be renewable rather than depleting whenever technically and economically practicable.

8. **Reduce Derivatives –** Unnecessary derivatization (use of blocking groups, protection/deprotection, temporary modification of physical/chemical processes) should be minimized or avoided if possible, because such steps require additional reagents and can generate waste.

9. **Catalysis –** Catalytic reagents (as selective as possible) are superior to stoichiometric reagents.

10. **Design for Degradation –** Chemical products should be designed so that at the end of their function they break down into innocuous degradation products and do not persist in the environment.

11. **Real-time analysis for Pollution Prevention –** Analytical methodologies need to be further developed to allow for real-time, in-process monitoring and control prior to the formation of hazardous substances.

12. **Inherently Safer Chemistry for Accident Prevention –** Substances and the form of a substance used in a chemical process should be chosen to minimize the potential for chemical accidents, including releases, explosions and fires.

[1]Green Chemistry at a Glance . (n.d.). American Chemical Society. Retrieved August 8, 2013, from http://www.acs.org/content/acs/en/greenchemistry/about/green-chemistry-at-a-glance.html

2151 Tentative ACS Fall Schedule

August

29 2014-2015 Officer's Meeting

September

5 Welcome Back – with Pizza

12 All About Career Services
with TBA

19 The Pre-Professional Timeline
with Ms. Andrea Abt

26 The Hows and Whys of Graduate School
with Professor Steve Weber

October

3 Fall Term Birthday Celebration

10 Meet Our New Faculty
with Professor Peng Liu

17 Preparation for National Chemistry Week

24 Pumpkin Painting

31 Chemistry at PPG
with Autumn Blackburn, B.S. University of Pittsburgh

November

7 Food Chemistry at Hershey
with Tara Kennedy, B.S., University of Pittsburgh

American Chemical Society

Student Affiliates, University of Pittsburgh

Membership Application

This is a powerful professional organization for the benefit of individuals interested in chemistry and related fields. Our organization offers exciting extracurricular activities and many outstanding opportunities for our members, including:

1. **WEEKLY MEETINGS**-to plan activities, provide interesting speakers, discuss ideas, and keep students aware of what is happening in the scientific community.

2. **ANNUAL TRIPS**-Each year we sponsor (a) trip(s), to external chemistry environments, as well as for social enjoyment. Significantly reduced rates are available to active members. In the past few years we have traveled to New Orleans, Atlanta and New York.

3. **PROFESSIONAL NETWORKING**-Our organization has many opportunities to make contacts with professionals in both the scientific industry and academia. Student affiliates also have the opportunity to join the National ACS.

4. **SOCIAL ACTIVITIES**-We sponsor many activities throughout the year just for fun.

Our meetings are held every Friday at 12:00 noon in Room 135 Chevron Science Center. To join, complete the application form below and come to one of our meetings. Our first meeting will be <u>September 5, 2014</u> but you may join any time throughout the year.

Name: ______________________________

School Address: ______________________________

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Permanent Address: ______________________________

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School Phone: ____________________ Home Phone: ____________________

Major: ____________________ Year in School **Fr.** **So.** **Jr.** **Sr.**

E-mail: ______________________________

May we include your name, number and e-mail on the published phone list? **YES** **NO**

To submit this form by mail, send it to ACS-SA, Box 24, Chevron Science Center, University of Pittsburgh, Department of Chemistry, Pittsburgh, PA 15260. Be sure to include the $15.00 dues <u>(make checks payable to the University of Pittsburgh)</u>. It is possible to be active even if you can not attend the meetings. For more information, see our display case in the lobby of Chevron Science Center.