

Silicon Valley Chemist

Santa Clara Valley Section

American Chemical Society

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MARCH 2010 NEWSLETTER TOPICS

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April Dinner Meeting

Using Computers to Read Scientific Literature

Dr. Steven Boyer

Abstract:

We successfully use text analysis technology to identify chemical names and other entities in unstructured text. Once identified, we convert the chemical names into their chemical structures using [name=structure] programs. This produces simplified molecular input line entry specification (SMILES) strings representing the chemical structures, which are subsequently used in computational calculations and as input for other applications. Using this technology, we analyze millions of patents and Medline abstracts and generate a large database of molecular structures derived from the text of those documents. In addition to extracting chemical structures from the text of documents, we also exploit image analysis to selectively recognize the chemical images contained in documents and convert these images to SMILES strings. This work (text and image analysis) effectively renders the scientific and patent literature searchable by structure/substruc-

ture search applications. The combined technologies for reading and processing molecular structures allow researchers the ability to build large databases of previously inaccessible literature – relevant in the areas such as patents, pharmaceuticals, publishing, health care, and environmental science.

Integration of these and other operations has enabled us to process over 11 million documents to date with IBM's BlueGene supercomputer. We currently index over 100,000 documents per

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April Dinner Meeting

Date: Thursday, April 15, 2010

Time: 6:00 Social Hour
7:00 Dinner
8:00 Presentation

Location: Biltmore Hotel & Suites
2151 Laurelwood Blvd.
Santa Clara, CA 95054

Speaker: Dr. Steven Boyer
(co-inventor of the Delphion patent database)
Computers in Chemistry

Cost: \$27.00 with a choice of:
Teriyaki Steak
Vegetarian Lasagne

Reservations: www.scvacs.org or
Shirley Radding 408-246-2564
408-296-8625 Fax

Reservations should be made by April 12th stating your name, address, company affiliation, number of people in party, and menu selection. If you are unable to honor your reservation and do not cancel by Tuesday, April 13th, you will be invoiced following the dinner meeting.

Chair's Message

The big event in March is the National ACS Meeting in San Francisco, March 21-25. In cooperation with California Section, we are presenting posters in the meeting areas that tell about innovative chemists who have contributed to science and society.



The Synopsis Silicon Valley Science and Technology Championship will be held in the San Jose convention Center on Wednesday, March 17. Sign up to be a judge; you will find it fun and interest-

ing to meet with these students.

Ah, the memories of chocolate! Howard and Sally Peters gave a most interesting talk at our Mosher Award presentation in January. Thank you, Howard and Sally. If you didn't attend you missed tasting the many

chocolate samples.

Just a reminder about this month's program on Thursday the 18th. We will hear Dr. Joseph Castellano talk about energetic molecules and Russian spies.



April Dinner Meeting, continued from front page
month including all of the US, EP and WO documents on a weekly basis. Additionally, our computing environment is capable of indexing about a billion web pages in approximately 3 hours, retrieving and indexing biologically relevant information.

Biography:

Steven Boyer holds a Bachelor of Arts degree from Temple University in Philadelphia and a Ph.D. in synthetic organic chemistry from Tufts University in Massachusetts. He is married and has two children.

An Award for Mentoring in Science

According to a press release from Stanford University, chemistry Professor Richard Zare was at the White House recently to pick up an award for mentoring in science.

Zare, the Marguerite Blake Wilbur Professor in Natural Science, was one of 22 nationwide recipients of the Presidential Award for Excellence in Science, Mathematics and Engineering Mentoring.

"The amazing thing about Zare is his talent to explain complex theory in a very simple way," said Thomas Perroud, a former teaching assistant in Zare's lab. Perroud is now a senior member of the Biosystems Research and Development Staff at Sandia National Laboratories in Livermore.

"He uses analogies that are not only simple to understand but easy to remember, and he makes it very enjoyable, very lively," Perroud said Thursday.

The annual award, administered by the National Science Foundation, recognizes mentors who give their time, encouragement and expertise for the academic and personal development of science or engineering students who are minorities in their fields. Colleagues, administrators and students nominate candidates who mentor students of any grade level, from elementary through graduate school.

President Obama praised the educators for their passion and expertise in preparing students "to tackle the grand challenges of the 21st century such as increasing energy independence, improving people's health, protecting the environment and strengthening national security."

"The quality of math and science teachers is the most important single fac-

tor influencing whether students will succeed or fail in science, technology, engineering and math," he said.

Perroud said Zare "likes to bring students down to do chemistry demonstrations. He likes to make a mess. He likes people to participate."

He recalled a lunch with Zare and a group of undergraduates where people were drinking soda.

"He just started telling us about the chemistry of it, about sparkling water and lemon," Perroud said.

"Chemistry is basically everywhere in his life, not just in the classroom. He thinks of chemistry all the time and that allows him to translate the scientific and academic to life outside the classroom, outside the rigorous protocols," he said.

When Zare became chairman of Stanford's chemistry department, Perroud recalled, he created new policies for female students who became pregnant.

"He made a policy that she could have time off, and provided a framework so she could feel comfortable with balancing her personal life and her professional career. That was definitely a very good idea."

Zare is known for his work in laser spectroscopy, having developed a laser-induced fluorescence method that is widely used in chemistry laboratories. Laser induced fluorescence is the process of studying molecules by exciting them with a laser and then measuring the light they emit.

Zare joined the Stanford faculty in 1977, following undergraduate and graduate education at Harvard University, and working at the Massachusetts Institute of Technology, the University of Colorado and Columbia University.

He has over 25 years of experience in numerous capacities in corporate settings, first in the pharmaceutical environment and then in the computer world. With a Ph.D. in chemistry, Steve has found himself in a full spectrum of work places, from synthesizing drugs "at the bench" to launching the world's first public patent website. At IBM's Research Division, Steve is credited with being the "father" of the IBM Patent Server. This effort (1994-2000) aggregated the entire intellectual property of the world into a single database made available on the internet, a revolutionary act in its time. It resulted in one of the largest and most successful public information internet sites at that time on the web, a pivotal event that impacted the world of intellectual property (IP). As a result Steve served as an advisor to the World Intellectual Property Organization (WIPO) on the creation of WIPO-Net, an initiative to provide IP resources to third world countries, lecturing on technical issues and drafting proposals for improving international access to intellectual property. The IBM Patent Server was so successful that IBM spun it off as an independent business venture, Delphion (www.delphion.com), later acquired by Thomson Publishers.

At IBM, Steve has worked in numerous capacities, technical and managerial, including four years in Europe directing scientific and technical computing initiatives. His own recent patents apply computer technology to developing tools for building scientific databases and include internet metacrawling and searching technologies. His most recent activity has been in "text and image analytics", specifically on the automated annotation of large document repositories.



Reminder March Dinner Meeting Reminder

Energetic Molecules and Russian Spies

Dr. Joseph A. Castellano

Abstract:

This talk will discuss some of the government classified research on the synthesis and properties of nitrogen-fluorine compounds that was performed in the early 1960s at the Thiokol Chemical Company in Denville, New Jersey. Some of the reactions involving difluoramino (HNF_2), tetrafluorohydrazine (N_2F_4), and perfluoroguanidine (PFG) with various substances will be described. The objective of the research was to synthesize organic compounds with a large number of difluoramino (NF_2) groups for use in rocket propellant formulations. The higher the number of these groups per molecule, the more "energetic" the material. Formulas and samples of some of these materials were given to a Soviet KGB agent by one of our coworkers, code named "Cook," by the KGB. The story of this espionage activity and the ultimate fate of Cook as well as his KGB "handler" will also be related. Finally, some possible future uses



for nitrogen-fluorine compounds will be proposed.

Biography:

Joseph A. Castellano was born in Manhattan and raised in Brooklyn. He received his B.S. from the City College of New York (CCNY) and a Master of Science and Ph.D.

from the Polytechnic Institute of New York University (formerly the Polytechnic Institute of Brooklyn).

Castellano began his professional career in 1959 with the Witco Chemical Company in Paterson, New Jersey developing analytical methods for industrial chemical manufacturing. In 1962, he joined Thiokol Chemical Company, Denville, New Jersey, where he performed classified rocket fuel research under contract to the U.S. Naval Research Laboratory. Castellano joined RCA Laboratories in Princeton, New Jersey in 1965 and performed pioneering research in liquid crystal materials and electronic displays. He was a member of the team that developed the world's first

liquid crystal display (LCD). In 1976, he founded Stanford Resources in San Jose, California and as CEO helped grow the company into a world leader in market research and analysis of the electronic display industry. He retired in 2003 following the merger of Stanford Resources with iSuppli Corporation.

Castellano has authored or co-authored more than 60 scientific/technical papers and two books, and he is the holder of 12 U.S. patents. He continues to be active in several international scientific associations and helps teach eighth-grade physical science as a volunteer in the RESEED Silicon Valley program.

March Dinner Meeting

Date: Thursday, March 18, 2010

Time: 6:00 Social Hour
7:00 Dinner
8:00 Presentation

Location: Biltmore Hotel & Suites
2151 Laurelwood Blvd.
Santa Clara, CA 95054

Speakers: Dr. Joseph Castellano
Energetic Molecules and
Russian Spies

Cost: \$27.00 with a choice of:
Greek Chicken with olives
and feta cheese
Vegetarian Crepes

Reservations: www.scvacs.org or
Shirley Radding 408-246-2564
408-296-8625 Fax

Reservations should be made by March 15th stating your name, address, company affiliation, number of people in party, and menu selection. If you are unable to honor your reservation and do not cancel by Tuesday, March 16th, you will be invoiced following the dinner meeting.

UC Berkeley Extension Embraces Green Chemistry

As the demand for hazard-free products and production processes continues to rise, so does the need for skilled professionals in the field of green chemistry. Poised to meet those needs in the Bay Area and beyond, UC Berkeley Extension offers two new green chemistry courses this spring: Green Chemistry Policy (starting online February 9 and in Berkeley February 24) tackles the current and historical context of the regulation of industrial chemicals; Toxicology and Risk Assessment (starting in Berkeley Wednesday, March 31) examines the toxic effects of hazardous chemicals on biological systems. Both courses are part of the Certificate Program in the Essentials of Green Chemistry to be launched in late 2010 or early 2011 in both online and classroom formats.

To build excitement for these courses and the upcoming professional certificate,

Extension invites the public to attend a free lecture with Dr. Robert Peoples, director of the ACS Green Chemistry Institute. In "Can We Achieve a Sustainable Future? The Role of Green Chemistry," Peoples leads a lively dialogue about green chemistry's role in not only weaning modern society off petroleum but also tackling the challenges of global sustainability. Sustainability at its core means survivability, and green chemistry hopes to ensure that the global population is happy, healthy, and here in the future. This free public lecture takes place on Thursday, March 25, 6:30–8 p.m., in 105 Stanley Hall on the University of California, Berkeley, campus.

To learn more about UC Berkeley Extension's green chemistry offerings and to enroll, visit <http://extension.berkeley.edu/subject/chemistry.html>.



Volunteers Needed – 2010 Chemistry Olympiad

The 42nd International Chemistry Olympiad will be held in Tokyo, Japan, July 19-28, 2010. The US will be sending a team of four high school students to participate with students from 50 countries from around the world. Those four students will be selected from a pool of 20 outstanding students from across the United States.

The selection process begins right here in our local section! Chemistry students from the Santa Clara Valley will participate

by taking a standardized ACS written exam to determine their placement. The first round of testing is conducted in the high schools in March. The local section encourages the high schools to participate and provides the testing materials. Each school that participates will receive a gift copy of the Merck Index that was donated by Merck and the ACS.

The top 17 students will meet on Saturday, April 24th, to compete in the

national exams. About one thousand students from across the country will be taking the same exam that weekend. More written tests and a lab exercise will be administered at Las Positas College in Livermore. Students from the California section will join us for the day. The California section hosts the students and proctors that day and provides snacks and lunch.

Those exams are sent to national ACS for grading. The top 20 students are chosen from the 1000 participants. Those 20 will attend the weeklong study camp at the Air Force Academy in Colorado. Our section has been represented at the study camp in 2002, 2005 and 2007. The team that will represent the US in Tokyo is chosen on the last day of the study camp.

Would you like to help with the process? Encourage your local high school chemistry teachers to have their advanced placement and honors students participate in the testing process. We have over 100 high schools in the valley, but only about 15 compete. We contact each chemistry teacher and high school by letter in January, giving them the Olympiad information and encouraging them to participate.

A few local section members are needed to register the students and proctor the exams on April 24th at Las Positas College. This is an excellent chance to volunteer and encourage these students to think about careers in chemistry. It is an especially good chance for members who live in the East Bay! Lunch is even provided.

Also, if someone has access to a good color printer or scanner/printer, they could help by customizing the ACS student certificates that each student receives. Or, customizing by calligraphy would be grand! There should be about 150 certificates that will need to be customized.

So here are some opportunities to help your local section with the 2010 International Chemistry Olympiad – encourage the teachers to participate (maybe even offer to help them grade the exams!), volunteer to be a proctor, or help print certificates. If you need more information, please contact me.

Sally Peters

Chair of the Santa Clara Valley Section
Chemistry Olympiad Committee
Sally.Peters@parc.com
650-854-4614

Starting This Month and Thereafter

Welcome to the Santa Clara Valley Section of ACS

Each month the section receives a spreadsheet from national ACS with the names of members new to our section. The members are either new to ACS, have transferred in from other areas, or are the newest members -- the students.

To welcome you to the section and get to know you, the Executive Committee offers new members a free dinner!! To encourage you to attend a monthly section dinner meeting, we would like you to be our guest. When you register, make certain to mention that you are a new member and you and a spouse (or friend) will be our

guests. The dinner meetings are often the 3rd Thursday of the month at a local spot, somewhat convenient to the entire section.

If you are unable to attend in the evening, perhaps you would join us for an outreach event, like judging a science fair, participating in the chemistry olympiad, or a national chemistry week event in October. Then there is our annual wine tasting and awards picnic in July.

The local section is a volunteer organization. Please attend an event, volunteer to help, and get to know your local fellow chemists. Welcome!!

New Members List for March

Mr. Brian Aguado	Dr. Darin James Gustin
Mr. Jonathan Bakke	Ms. Jennifer Hensel
Christopher Barnett	Zach Hogan
Shawn Bauer	Mr. Brian Horvath
Ellen D. Beaulieu	Ying Hu
Lijing Chen	Dr. Maria Hutchins
Mr. Zhebo Chen	Dr. Richard Jack
Hiufung V. Chu	Mr. Douglas Jones II
Miss Chia-Jung Chung	Gregory J. Kearns
Maura T. Corcoran	Dr. Joshua Kennedy-Smith
Barthelemy Demeule	Ms. Eun Ah Kim
Dr. Stephen P. Dudek	Anna Le
Nigama Ekkad	Dr. Yitmin Liang
Mr. Abraham El Gamal	Yu Lin
Mr. Honghan Fei	Dr. Marcus Lundberg
Dr. Kelly Flook	Dr. Peter Madrid
Mathieu Frenette	John Mao
Dr. Alexandre Fuerstenberg	Mr. Bryan McCloskey
Alexander C. Gagnon	Dr. Tissaphern Mirfakhrai
Mr. Mark Garcia	Ms. Katherine Vanessa Nelson
Crystal Y. Gonzalez	Kim Nguyen
Dr. Girish Gopalakrishnan	Mr. Vincent Tien Nguyen
Yelena Gorlin	Dewi Nilasari
Michael Gottschalk	Ms. Munzarin Qayyum

Xuelei Qian
Ms. Nicole Romano
Mr. Michael Rowell
Dr. William Douglas Sands
Lauren Sartor
Dr. Thomas Scherer
Emilee Sena
Himanshu Sharma
Ms. Lauren Sirois
Dr. Lei Sun
Samuel Tan
Brian Trantow
Dr. Sebastien Ulrich
Ms. Diana E. Voigts
Mr. K. C. Wang
Shibing Wang
Dr. Y. John Wang
Nicholas John Ward
Dr. Anita Wu
Dr. Jessica Wu
Dr. Xunyu Yang
Dr. George Yi
Elena Zavala
Dr. Yan Zhao

Local Science Fairs in 2010

Contact: Howard Peters, peters4pa@sbcglobal.net

January to June of each year is the time for intense effort for IMPORTANT science and engineering fair competitions at the local, regional, state and international levels.

Monterey County Science and Engineering Fair

County High School students

Judges needed: Saturday, March 6, 2010

Location: California State University, Monterey Bay.

For more information, visit www.montereycountysciencefair.com/

Santa Cruz Science Fair

Santa Cruz County high school students

Date: Saturday, March 13, 2010

Location: Santa Cruz Civic Auditorium, Santa Cruz

For more information, visit www.science.santacruz.k12.ca.us/links.html

Synopsys Championship (aka Santa Clara Valley Science and Engineering Fair)

Date: Wednesday, March 17, 2010

Location: San Jose Convention Center, San Jose

For more information, visit www.outreach-foundation.org/judges.html

San Francisco Area Science Fairs - ISEF affiliate

San Mateo County students eligible

Judges needed: Thursday, March 25, 2010

Location: San Francisco County Fair Ground Building - Golden Gate Park

Contact: Greta Mayfield (925)842-3047 or Greta.Mayfield@chevron.com

For more information, visit www.usc.edu/CSSF/Fairs/300.html

Tri-Valley Science and Engineering Fair

Date: March 30-April 2, 2010

Location: Livermore CA

For more information, visit: <https://tvsef.llnl.gov>

Intel International Science and Engineering Fair (ISEF) World Class Competition

Date: Sun-Fri May 9-14;

JUDGING Tues-Wed, May 11, 2010 5pm to 8pm and
May 12, 2010 from 8am to 6pm.

Location: San Jose Convention Center, San Jose CA

Contact: Dr. Howard Peters at peters4pa@sbcglobal.net
or Dr. Roy Okuda, SJSU at okuda@sjsu.edu.

For more information, visit: www.sciserv.org/isef/ or
www.isef2010sanjose.org/judges.html

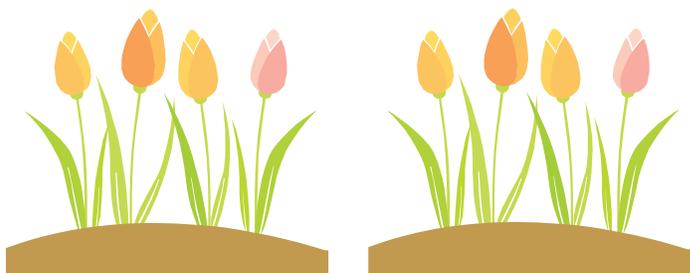
California State Science Fair

Date: Monday-Tuesday, May 17-18, 2009

Location: California Science Center, LA.

For information, visit: www.usc.edu/CSSF/

For other affiliated U.S. Science Fairs, please visit: www.societyforscience.org/



JOBS! JOBS! JOBS!

**Employers Are Looking to Hire:
If You Are Looking for a Job,
Register for the ACS Career Fair!**

The Career Fair is the premier place where employers can promote their company and meet job seekers face-to-face to discuss employment opportunities. Job seekers can attend a variety of workshops, participate in mock interviews, and make appointments for individual résumé reviews. The Career Fair will be located in the Moscone Center, West Hall, Level One. It will be held Sunday, March 21, 10 am to 5:30 pm; Monday and Tuesday, March 22-23, 8 am-5:30 pm; and Wednesday, March 24, 8 am-noon. Job seekers and employers can register at www.acs.org/careers.



SEE the Future of Sustainability through Chemistry

The global challenges of providing sufficient and secure energy, clean drinking water, and adequate food, housing, and medical care will require the creative input of all of the planet's scientists. To address these challenges, ACS will host an innovative Sustainability Engagement Event (SEE) during the spring national meeting in San Francisco (www.acs.org/sustainability).

The event will help us to SEE this future. It will focus on collecting, refining, and implementing the ideas of a broad range of stakeholders, and on strengthening their engagement. The goals are to generate excitement about the ACS sustainability efforts; to brainstorm, create, and develop projects that can and will make a difference; and to connect with members of all ages and fields, especially those who are not currently engaged with ACS on a volunteer level.

The varied backgrounds and experi-

continued on next page

SEE the Future, continued from previous page

ences of chemists inspire us in different ways to offer workable solutions at the local, regional, and global levels. Working together, ACS and chemists can identify the solutions that will help us achieve a sustainable future.

All meeting attendees and ACS members are invited to participate in the event forum. Even if you are not planning to be in San Francisco, you are encouraged to share your ideas at www.acs.org/sustainability. The SEE kickoff will take place on

Sunday, March 21 from 6 to 8:30 pm in the Expo Hall, and the forum will be on Tuesday, March 23 from 3 to 5:30 pm. Preregistration is requested for the forum, which is quick and easy at www.acs.org/sustainability.

Speak for Science

Less than 10% of the 535 members of Congress have backgrounds in science and engineering. Yet every day, legislators are asked to make important decisions that affect our nation's scientific enterprise. You and your committee members can help them make informed decisions by joining the ACS Legislative Action Network (LAN).

The LAN is a Web-based political involvement program that gives you an easy, effective way to voice opinions on legislation effecting federal research to K-12 science education.

As you may know, for decades ACS has been a respected source of information and advocacy on Capitol Hill. Often

this input is provided in formal testimony before committees and panels making decisions on spending and legislation relating to science and engineering.

But just as important, members of Congress listen to their constituents and value their timely input. That's where you and your committee members can play a valuable role as members of the LAN.

Prior to key congressional decisions, ACS staff sends e-mail alerts to LAN members with background information, the analysis of the potential effect an issue would have on the scientific enterprise, and ACS's position. By clicking on a Web link, participants can go directly to the ACS Legislative Action Center, where

they are given background information on the topic and a proposed message that can be easily personalized and sent directly to legislators—the entire process takes only a few minutes.

It's free, simple, and done entirely via the Web. But more to the point, by participating in the LAN, chemists can impact federal policies critical to chemistry and our nation. Please register online at www.act4chemistry.org/register.cfm.

If you would like more information on the Legislative Action Network, please contact the ACS Office of Public Affairs at 1-800-227-5558, ext. 4386, or b_smith@acs.org. Participate and become your legislators' "face of science."

CHEMPLOYMENT ABSTRACTS MARCH 2010

CHEMPLOYMENT ABSTRACT 3947

Position Title: Research Associate - Medicinal Chemistry

Job Description: The Research Associate - Medicinal Chemistry will participate in Genentech's innovative program in drug discovery. The candidate will be responsible for the design and synthesis of novel drug-like compounds.

QUALIFICATIONS DESIRED:

Education: Bachelor's or Master's degree in Organic Chemistry

Experience: This position requires 2-8 years of experience in synthetic or medicinal chemistry. The incumbent should be highly motivated and excited to work in a collaborative environment. Demonstrated expertise in multi-step synthesis, compound purification and structural characterization is preferred.

LOCATION, SALARY, EMPLOYER DESCRIPTION:

Job Location: South San Francisco, CA

Salary: DOE

Employer Genentech is among the world's leading biotech companies, with multiple therapies on the market for cancer and other serious medical conditions

Application Instructions: Genentech is dedicated to fostering an environment that is inclusive and encourages diversity of thought, style, skills and perspective. To learn more about our current opportunities, please visit: <http://careers.gene.com> and reference Req. #1000030386. Please use "Web - ACS" when a source is requested. Genentech is an equal opportunity employer



Photos from the January 21st Mosher Award to Howard and Sally Peters

By Lois Durham



Grace Baysinger, Peter Rusch and Sally Peters



Natalie and Jim McClure, Peter Rusch



Jim and Ro Dinkey



Roy Okuda and Maureen Scharberg



Bruce Raby



Sally Peters



Howard Peters



Natalie McClure



Natalie McClure, Sally Peters, Carol Mosher and Howard Peters



Frank Dennis, Grace Baysinger and Mark Kent



Ida Raby, Marjorie Ottenberg and Bob Wallace



Than-Ngoc Le, Oliver Olivero and Howard Peters



Mark Kent and Carol Mosher



SANTA CLARA VALLEY SECTION
AMERICAN CHEMICAL SOCIETY
P.O. Box 395, Palo Alto, CA 94302

Visit our web site at:



<http://www.scvacs.org>

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is published on our web site, sign up at:
<http://www.scvacs.org/newsletter/>

SANTA CLARA VALLEY SECTION

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Secretary	Karl Marhenke	831-688-4959	karlmar@armory.com
Treasurer	Ihab Darwish	650-594-1654	darwishis@yahoo.com

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ChemPloyment Abstracts

Director	Charles Sullivan	650-728-7034	cdansullivan@sbcglobal.net
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FUTURE MEETINGS

- Mar 12-14** Santa Cruz County Science Fair
<http://science.santacruz.k12.ca.us>
- Mar 17** Synopsys Silicon Valley Science
and Technology Championship
San Jose Convention Center
www.outreach-foundation.org
- Mar 18 Meeting** Dr. Joseph Castellano
Energetic Molecules and Russian
Spies
- Mar 21-25** Spring National Meeting
Chemistry for a Sustainable World
San Francisco, CA
- Apr 15 Meeting** Dr. Steven Boyer
Using Computers to Read Scientific
Literature
Santa Clara, CA
- Apr 24** Regional High School
Chemistry Olympiad
Las Positas College, Livermore, CA
- May 9-14** Intel International Science and
Engineering Faire
San Jose Convention Center
www.societyforscience.org/ISEF