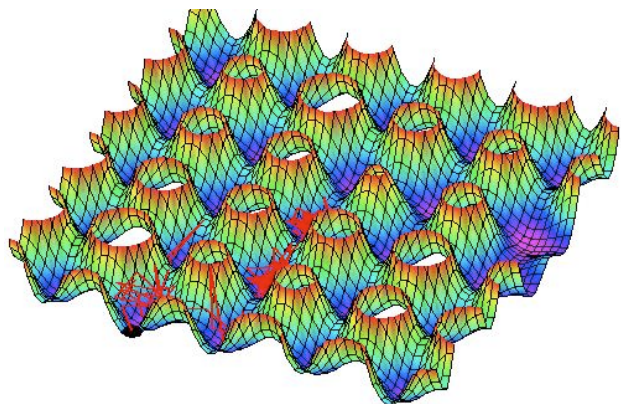




THE OCTAGON

838th LVACS Meeting:
January 22, 7-9 PM - Webinar



Pulling proteins apart on a computer: How and Why? **Rigoberto Hernandez, Georgia Institute of Technology**

The behavior and function of proteins necessarily occurs during nonequilibrium conditions such as when a protein unfolds or binds. The high-dimensionality of these systems—because of the large number of atoms in the proteins and their environments—presents significant challenges to theoretical or computational methods. The present work attempts to reign in this complexity by way of capturing the dominant energetic pathway associated with a chosen structural transition of the protein. In particular, the energetics of an unfolding event can be formally obtained using steered molecular dynamics (SMD) and Jarzynski's inequality but the cost of the calculation increases dramatically with the length of the pathway. An adaptive algorithm (ASMD) has been introduced¹ that allows for this pathway to be nonlinear and staged while reducing the computational cost. The potential of mean force (PMF) obtained for neuropeptide Y (NPY) in water along an unfolding path confirmed that the monomeric form of NPY adopts the pancreatic-polypeptide (PP) fold. ASMD can also be used to reconstruct² the PMF obtained earlier for

stretching decaalanine in vacuum³ but at lower computational cost. The PMF for stretching decaalanine in water solvent (using the TIP3P water potential) at 300K has now been obtained using adaptive SMD.⁴ Not surprisingly, the stabilization from the water solvent reduces the overall work required to unfold it. However, the PMF remains structured suggesting that some regions of the energy landscape act partially as doorways. This is also further verified through a study of the hydrogen-bond breaking and formation along the stretching paths of decaalanine in vacuum and solvent.

References

- ¹G. Ozer, E. Valeev, S. Quirk and R. Hernandez, *J. Chem. Theory Comput.* **6**, 3026-3038 (2010).
²G. Ozer, S. Quirk and R. Hernandez, *J. Chem. Phys.* **136**, 215104 (2012).
³S. Park and K. Schulten, *J. Chem. Phys.* **120**, 5946 (2004).
⁴G. Ozer, S. Quirk and R. Hernandez, *J. Chem. Theory Comput.* **8**, 4837-4844 (2012).

MEETING DETAILS:

January 22, 7-9 PM -Webinar hosted by Penn State Berks. Space is limited.

Reserve your Webinar seat now at: <https://www3.gotomeeting.com/register/363867534>

A confirmation email with instructions will be sent. System Requirements: Windows® 7, Vista, XP or 2003 Server; Mac OS® X 10.5 or newer;; iPhone®, iPad®, Android™ phone or Android tablet

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839th LVACS Meeting: *Wednesday February 13*

Muhlenberg College

Reception: 5:30; dinner following

Meeting: 7:00

RSVP LuAnn Feist, 484-6643260,
feist@muhlenberg.edu by 5pm

Thursday February, 7th



PROGRAM INFORMATION:

SPEAKER: Dr. Chriss McDonald of Lycoming College

TOPIC: Novel Samarium Diiodide-Based Reduction Systems

Speaker: Dr. McDonald graduated with a B.S. degree in medical technology from Manchester College (IN). He then earned a Ph.D. in organic chemistry from Miami University (OH). After one year as a sabbatical replacement at Berea College (KY), he obtained a tenure track appointment at Lycoming College (PA). He currently holds the position of Professor of Chemistry at Lycoming. His research interests include radical synthetic chemistry and the development of novel inquiry-based experiments for the undergraduate organic chemistry laboratory.

ABSTRACT:

The goals of this project are two-fold:

- 1) To find activators for samarium diiodide (SmI_2) that exclude known mutagenic moieties, such as the *N*-methyl groups found in the most common activator, HMPA ;
- 2) To identify compounds which are better activators of SmI_2 than HMPA. Multiple compounds have been identified which accomplish these goals. Efforts to characterize the complexes (kinetic, cyclic voltammetry, X-ray analysis, UV-vis) formed between these compounds and SmI_2 , and comparison to the analogous complex formed between SmI_2 and four HMPA molecules, will be discussed. The use of these complexes in important synthetic transformations will also be addressed.

MEETING DETAILS:

Further details including location details, directions and menu will be posted on the website as soon as they become available.



A MESSAGE FROM THE CHAIR

Greetings LVACS Colleagues,

Welcome to a new year of the Lehigh Valley Section of the American Chemical Society. The last time I had the privilege of serving this superb section, I was your Secretary in 2002 and 2003, Chair-Elect in 2004, and Chair in 2005. I spent some time reminiscing via documents and minutes from those years. In 2005, Richard Schrock, Robert Grubbs, and Yves Chauvin received the Nobel Prize in Chemistry for their work in the area of olefin metathesis (an organic synthesis technique). Our collective scientific genres lost the likes of Frances Crick, John Clark, and Julius Axelrod, three of several inspiring and influential professional persons. This was also the time I was transitioning between laboratory research and clinical research, and had my big introduction to the world of public relations with the withdrawal of Vioxx, occurring the day of our combined meeting with the Philadelphia Section at Merck's West Point Research site (September 2004). A combination of events and influences culminating in my decision to pursue my PhD in biochemistry while continuing my work in clinical research. I was not as active in LVACS as desired during those years, and I am happy to return and serve you again as Chair for 2013.

Technology has allowed us to once again have our January meeting via teleconference. We will reconvene face-to-face in February at Muhlenberg, and then enjoy High School Teacher's Night at DeSales in March. Cedar Crest College will host our annual Student Poster Session in April, and we are working on some exciting and interesting ideas for our traditional "casual" May meeting. Chester Crane will continue his excellent work at coordinating the Iron Pigs game in the summer.

Please feel free to introduce (and re-introduce!) yourself to me, and the entire Executive Committee. Ask us what we do,



provide suggestions to help improve the section. I think about all the conversations from members at meetings years ago during my time on the Executive Committee, and I see the return on the investment that each participating member provided. We have a great section (our ChemLuminary Award is one result of our hard work); we will make it better with your help.

Think about serving. Think about running for an office, or volunteering for a Committee Chair position. The best way to find out about these opportunities is to ask us! We will excite you about becoming more involved in LVACS. Find out: how do we fit this into "life"? Do we like it (yes, of course we do, but how do we handle the challenges and frustrations that come with any volunteer service)? Why are we participating? Etc. etc. etc. I encourage anyone to participate at whatever level possible. Each person can make a difference, as the LVACS is successful because of YOU.

As always, we are here and will listen to your thoughts, ideas, and action plans for our section. We can learn and grow from one another. Think about what you want from this section, and how it can happen. Let's plan and do it!

I look forward to meeting and interacting with you. Blessings and Be Well.

Cheers,

Tara S. Baney, PhD, Chair LVACS

Email: tsbaney@gmail.com, Phone: 862-210-5813



Spring 2013 LVACS Meeting Schedule

March 22, 2013 DeSales University, High School Teachers' Night

April 16, 2013 Cedar Crest College, Undergraduate Student Poster Session

May - TBD

EARTH DAY 2013

Happy New Year!



I'm excited to participate in LVACS's activities as the immediate past chair in 2013. One of my favorite celebrations of the year is Earth Day, and it is my pleasure this year to serve as coordinator for that event. Earth Day was first officially recognized on April 22, 1970 as a way to demonstrate support for a healthy environment, raise awareness about environmental issues, and remind people that we all need to contribute to a sustainable planet.

This year will be the 10th anniversary of Chemists Celebrate Earth Day (CCED), when all four topics of water, air, plants/soil, and recycling will be covered. The theme is "Our Earth: Handle with

Care!". More news from ACS will be available later in January.

LVACS is happy to participate this year in the national illustrated poem contest for students in Kindergarten - 12th grade. We welcome area Kindergarten- 12th grade students to compete. Details about the format, mechanism for participation and prizes will be available in the February Octagon, and - shortly - at lvacs.net. I hope you will help us distribute this information in your community.

Are you already planning an activity? Please let me know so I can help publicize it! Nothing yet? Consider checking the ACS website for a list of other fun, easy-to-implement activities.

I look forward to working with you,
Lorena Tribe -CCED Coordinator -2013



PJAS NEEDS VOLUNTEER JUDGES

On **Saturday, February 23, 2013**, junior and senior high school students affiliated with the Pennsylvania Junior Academy of Science Region III will present their science, computer, and math projects at Easton Area High School in Easton, PA. Please consider donating your time and talent to serve as a judge of these presentations. **We need your help to promote the appreciation of science, technology, and math in today's young people. Help us provide a meaningful experience for them as they develop interest in these disciplines.** If you can judge or assist in any way, please contact Megan K. Basile at mbasile@stsd.org



LVACS STRATEGIC PLAN UPDATE

We are now 6 months into our 18-month development actions for our Strategic Plan, launched in May 2012. Of 11 strategy items, we have completed 3 and are tracking well to complete 6 more by the summer of 2013 and the remainder by the end of 2013. As you know, a key focus is to increase member involvement with a goal of reaching a level of 100 active section members (with active defined as participating in at least at least 3 section activities per year) in 5 years. This is a challenging goal for LVACS but we are confident that we can achieve it. Please consider becoming an active section member by joining one of our committees and getting involved in the fun!

- Nigel Sanders, Chair, Strategic Planning Committee

Strategy	Leader Team	Action Plan	Status 12/10/2012
Communicate volunteer activities in a timely and diverse manner	Kelley Caffin	Find a way to reach all LVACS members to let them know what is going on and how they can help	[completed]
Establish population density maps to hold local meetings/activities close to different groups of members	Tara Baney: Chester Crane	Find out where our LVACS members are located and how we can get closer to them	we have paper version - used for student networking meetings. Need to make this electronic. John Freeman will ask ESU geographer!
Steel Stacks Kick Off	Nigel Sanders	Kick Off our Strategic Plan at the May 2012 meeting	[completed]
Accurate email	Carol Libby	Obtain updated email addresses for LVACS members to make sure we are reaching them	[completed]
Recognition	Bill Miles. Nigel Sanders. Jeanne Berk	Establish Volunteer of the Month Award to recognize volunteers	Jeanne, Bill and Nigel will have a meeting to develop a list of candidates
Increase committee membership	Danielle Ringhoff: Sara Hayik	get 3 or more members on each committee (including chair)	Make 4 awards committees one. OK for now - revisit in 6 months. Strategic Planning needs one more member to pull together member participation data. Sara will set up an app to do this. THIS IS A KEY WAY TO TRACK MEMBER ACTIVITY.
Appoint institutional points of contact	Lorena Tribe. Greglynn Gibbe	Have a single point of contact at each institution that has more than 3-5 members	14 institutions now have contact (NEW people - not already involved in section activities). Target is "top 30" Greglynn has generated Google map of industries with employees in our section.
Public Speaker List	Roger Egolf	Have a ready list of speakers we can recommend for chemically related topics	Roger put a piece in the May 2012 Octagon and followed up with emails to some people - no response. Need a new approach: Roger will put out email blast to entire section.
Full Year Meeting Schedule	Tara Baney	Have the meeting schedule complete by the end of August each year	For 2013-14 we need to strive to meet the August 2013 goal for ALL meeting dates/speakers to be posted on the website and published in September Octagon.
Publish a regular Octagon	LVACS Web Team = Michelle Jones-Wilson + committee chairs	Establish consistent monthly schedules/process for obtaining materials/content for Octagon and website	Good so far this year - keep up the trend!!
Keep website up to date	Fan Kistler: Phil Weizer	Increase currency and diversity of LVACS website content	Schedule another web design session with Michelle. Do as a webinar with Michelle broadcasting from ESU and group at Cedar Crest.



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Get the Word Out!

Are you volunteering in your community? Do you have any upcoming chemistry or science events planned?

Help is available to help get yourself, your volunteers and your event spotlighted at your college and/or in the local and regional news. Contact the LVACS Public Relations Chair, Greglynn Gibbs, gdw104@psu.edu.

Nothing says "Thank You" like well deserved recognition!