



The Bulletin
of the
Virginia Section
AMERICAN CHEMICAL SOCIETY

OCTOBER MEETING NOTICE

**Mary Baldwin College
Staunton, Virginia**

Friday, October 21, 2005

SOCIAL HOUR: **5:30 p.m.**
Ballroom
Student Activities Center

DINNER: **6:30 p.m.**
Ballroom
Student Activities Center

PROGRAM: **7:45 p.m.**
Room 301
Pearce Science Center

MENU: Chicken Breast in Herbed Wine Sauce, Cheese-Filled Pasta Purses with Pesto, Spinach Salad with Strawberries Toasted Almonds and Home-Made Raspberry Vinagrette Roasted Red New Potatoes, Sautéed Vegetable Medley, Steamed Asparagus with Orange-Dill Butter, Rolls and Butter, Home-Made Pies and Cheesecake, Sweetened and Unsweetened Iced Tea

PRICE: Members /Guests - \$15.00; Students, High School Teachers, Retired ACS Members/Spouses, Retired Teachers/Spouses - \$8.00

DINNER RESERVATIONS: Please make reservations by **NOON** on Wednesday, October 19 by calling Mrs. Teri Maerki at (540) 887-7116

HOST: Dr. Elizabeth Hairfield, (540) 887-7117, bhairfie@mbc.edu

SPEAKER: **Dr. Matthew Neurock, University of Virginia**

TOPIC: **“From Computational Chemistry to Catalyst and Materials Design”**

OCTOBER 2005

S	M	T	W	T	F	S
						1
2	3	4	5	6	7	8
9	10	11	12	13	14	15
16	17	18	19	20	21	22
		<i>reservations</i>			<i>meeting</i>	
23	24	25	26	27	28	29
30	31					

Dr. Matthew Neurock

Matthew Neurock obtained his Ph.D. degree in Chemical Engineering from the University of Delaware in 1992. He subsequently went on to work as a Postdoctoral Fellow at the Schuit Institute of Catalysis at the Eindhoven University of Technology in the Netherlands. From September 1993 to December 1994, he worked as a Visiting Scientist in the Corporate Catalysis Center at the DuPont Chemical Company in Wilmington Delaware. He joined the faculty in Chemical Engineering at the University of Virginia in 1995 and is currently the Alice M. and Guy A. Wilson Professor of Chemical Engineering and in addition holds a joint appointment in the Department of Chemistry. His work is focused on the simulation of material properties and processes with a particular interest in catalysis. Matt received the 2005 Paul H. Emmett Award in Fundamental Catalysis from the North



American Catalysis Society and has also been the recipient of an NSF Career Development Award, a DuPont Young Faculty Award, a Ford Young Faculty Award, and a Distinguished Catalysis Researcher from Pacific Northwest Laboratory. Matt has published over 130 paper and holds two patents.

From Computational Chemistry to Catalyst and Materials Design

The chemical, electrical, magnetic, and catalytic properties of nanoscale materials are dictated by their specific atomic architectures that form upon synthesis or processing. An understanding of how the structure dictates the materials performance presents a critical challenge, as the atomic scale resolution of the surfaces of these systems has historically been difficult to establish. The tremendous advances in spectroscopy and computational chemistry that have over the past decade, however, are beginning to provide a more detailed understanding of atomic structure that forms at interfacial surfaces, nanoscale particles and bulk materials. Ab initio calculations combined with atomistic simulations can begin to provide a detailed understanding of the physicochemical processes which control the structure at the surface of these materials along with its reactivity and kinetics. Theory and simulation can also begin to probe new material systems and thus be used towards the design of new materials.

This talk will try to briefly summarize the current computational methods and demonstrate their application towards the “in-silico” design of different nanoscale material systems. More specifically we will focus on the design of heterogeneous catalytic systems to carry out different chemical conversions as well as electrocatalytic processes for fuel cell systems, along with the nanoscale design of processes for optimal magnetic thin films, hybrid inorganic-organic materials.

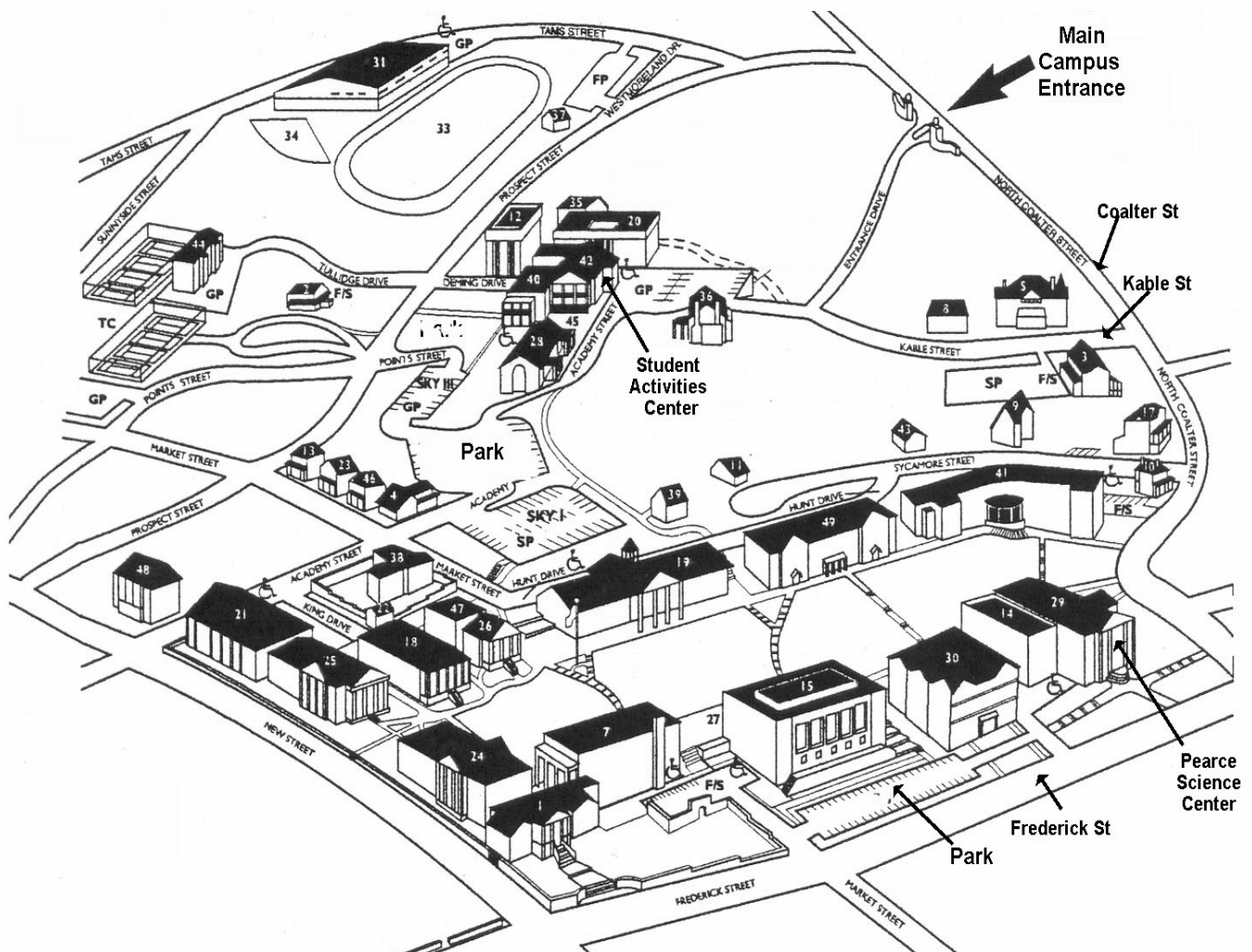
DIRECTIONS

From the East and South: I-64 West to Exit 87 to I-81 for 1/2 mile (East only). Take Exit 222, merge right onto 250 West. Go 2 miles; merge right at the fork in the road. Get into the center lane to go through the underpass. Proceed up the hill - you will see the College. Turn left onto Frederick Street or continue to Kable St (see Parking below).

From the North: I-81 to Exit 225. From the exit ramp, turn right onto Route 275 West. Turn left on Route 11 South. Bear right at the first fork (Route 11 Business). Bear left at the next fork (North Coalter Street). Pass the MBC hockey field and main entrance. Turn right on Kable Street or continue to Frederick Street (see Parking below)

Parking: Turn left onto Frederick Street; parking is available on your left. This parking is near Pearce Science Center; you will have to walk to the top of the hill for the dinner or turn left onto Kable Street. Proceed up the hill to the entrance to the upper campus. Parking is to the right or to the left down a short ramp.

MAP OF MARY BALDWIN COLLEGE CAMPUS



***** VIRGINIA SECTION NEWS *****

FUTURE MEETINGS

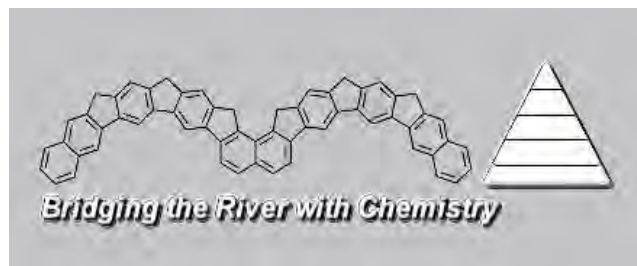
DATE: November 18, 2005	DATE: December 2, 2005
LOCATION: Mary Washington College Fredericksburg	LOCATION: Afton Research Center Richmond
HOST: Dr. Roy Gratz	HOST: Rob Davidson
PHONE: (540) 654-1412	PHONE: (804) 788-6327
SPEAKER: Dr. John J. Meister	SPEAKER: Dr. Kevin M. Dunn
TOPIC: "Your Garbage = My Reactants: Trash Recycling"	TOPIC: "Caveman Chemistry: Hands-On Projects in Chemical Technology" Presentation of Teaching Awards

SOUTHEAST/SOUTHWEST JOINT MEETING

The joint Southeast/Southwest regional meeting will be held at the Peabody Hotel in Memphis, Tennessee, November 1-4, 2005. Some highlights:

The Southern Chemist Award address:

Dr. James M. Tour of Rice University, "Nanotechnology's Active, Hybrid and Passive Applications. NanoCars, Hybrid Silicon/Molecule Electronics and Carbon Nanotube Composites" and an associated symposium.



Other special symposia include:

- Bioactive Lipids
- Biomedical Applications of Polymers
- Biosensors (sponsored by BD Technologies)
- NMR Spectroscopy and Structural Biology (sponsored by Bruker BioSpin)
- NMR Application in Metabonomics and Metabolomics (sponsored by Bruker BioSpin)
- Frontiers in Nucleic Acid Chemistry
- Guided Inquiry in the Chemistry Curriculum (CHED)
- Innovations in the Teaching of Chemistry (CHED)
- Chemistry and the Law
- Chemical Safety Inspections & Audits for Industry and Academia (CHAS)
- Nanomaterials and Composites: Synthesis, Properties and Applications
- Functionalized Metal Nanoparticles for Sensing Applications
- Spectroscopy and Chemistry of Matrix-isolated Species and Chemistry of Matrix-isolated Species

Workshops include:

- Laboratory Waste Management (CHAS)
- Laboratory Safety Management in Academia (CHAS)
- How to be a More Effective Chemical Hygiene Officer (CHAS)
- Thriving in the Workplace: An Awareness Program (ACS Younger Chemists Committee)
- How to Start a Co-op (ACS Undergraduate Programs)
- Process-Oriented Guided-Inquiry Learning (POGIL)
- Bruker BioSpin NMR Applications

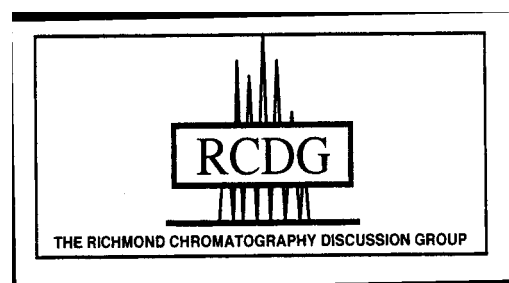
The exhibition will be open Nov. 2-3 and a college fair will be held on Nov. 4. For further information and updates on the Joint SE/SW Regional ACS Meeting Memphis-2005 visit online at <http://www.chem.memphis.edu/acs/seswrn.html>.

☞ NATIONAL CHEMISTRY WEEK
»»» OCTOBER 16 - 22, 2005 «««

“The Joy of Toys”
<http://www.chemistry.org>

RCDG

The Richmond Chromatography Discussion Group meets monthly for discussions of topics related to chromatography. For more information on RCDG or its meetings, or to have your name placed on their newsletter mailing list, contact Carol Sheets at (804) 358-9468, Csheets@aderis.com. Or check their website: www.rcdg.org.



SCIENCE FAIR WINNERS

The Virginia Section sponsors chemistry prizes at the Metro Richmond Science Fair. For the 2005 Science Fair, the first place prize in Chemistry was awarded to Katie Peng, a student at the Mathematics & Science High School in Chesterfield County. Katie received \$100 from the Virginia Section. The second place winner was Courtney Stephens who attends the Center for Science, Mathematics and Technology at Mills E. Godwin High School in Henrico County. Courtney received \$50. The Section also gave cash awards to the two high schools.

CHEMISTRY AT MARY BALDWIN COLLEGE

Mary Baldwin College is committed to the education of women for a world of expanding opportunity. We consider it one of our particular missions to prepare women for careers in fields that have been traditionally closed to them and to advance the careers of women who are presently in non-traditional fields. We provide a challenging, but encouraging, environment for students at all points of the age spectrum, from 13-year-olds enrolled in the Program for the Exceptionally Gifted (PEG), through traditional-age students in the regular undergraduate program, to mid-career professionals in the Adult Degree Program (ADP).



Much of the strength of our chemistry program arises from an emphasis on laboratory work, including student research. We want our students to know not only the theories of chemistry taught in the classroom but also the practical aspect of chemistry learned in the laboratory. All of our majors complete 8-9 credit hours of laboratory as well as a full year of senior research, including participation in a research seminar and the writing and oral defense of a thesis based on their work. Most of the majors also present their work before the Virginia Section of the American Chemical Society scholarly body.



The modern teaching and research laboratories are in the Pearce Science Center. Among other equipment, students can work with a scanning electron microscope; ultraviolet-visible, infrared (FTIR), nuclear magnetic resonance, and atomic absorption spectrometers; a high performance liquid chromatograph; a capillary gas chromatograph with FID detector; and a capillary gas chromatograph-mass spectrometer. College computers are available in Pearce as well as other academic buildings when students need them for their studies and for writing their theses.

SEMINARS AT THE UNIVERSITY OF VIRGINIA

- Oct. 14 - **Professor Rigoberto Hernandez**, Georgia Institute of Technology, "Control of Transport on Surfaces and Validation of Protein Structures"
- Oct. 21 - **Dr. Linda Columbus**, Scripps Research Institute, "Investigating Structure and Dynamics of Proteins with Magnetic Resonance"
- Oct. 28 - **Professor M. G. Finn**, Scripps Research Institute, "Chemically Tailoring the Form and Function of Virus Particles"
- Nov. 4 - **Professor Geert-Jan Boons**, University of Georgia, "Telling Glycosidase Inhibitors What to Do"

Nov. 18 - **Professor Lanny Liebeskind**, Emory University, "Organometallic Enantiomeric Scaffolds: An 'Organometallic Chiron' Approach to Asymmetric Synthesis"

Chemistry colloquia are held at 4:00 p.m. in Room 304 of the Chemistry Building. The complete colloquium schedule is on-line at <http://www.virginia.edu/chem/newsandevents/seminars/>.

SEMINARS AT VIRGINIA COMMONWEALTH UNIVERSITY

Thursday, October 13 - **Dr. Kostic**, Iowa State University

Thursday, October 20 - **Prof. Shekhar Garde**, Department of Chemical & Biological Engineering, Rensselaer Polytechnic Institute, "Water-mediated interactions relevant to protein structure and function"

Thursday, October 27 - **Dr. Jennifer Lewis**, Department of Chemistry, University of South Florida

Thursday, November 17 - Christopher Cahill, George Washington University

Tuesday, November 29 - **Prof. Trevor M Penning**, Department of Pharmacology, University of Pennsylvania, Aldo-keto Reductases and Polycyclic Aromatic Hydrocarbon Activation

Seminars are in the Kapp Lecture Hall, Room 1024, in the Mary E. Kapp Wing of Oliver Hall, 1001 West Main St., Richmond. Refreshments at 3:45 PM, Seminar at 4:00 PM.

For more information call (804) 828-1298.

QUESTION FROM THE PAST

Question from the September issue: When it was first chartered in 1915, the Virginia Section encompassed the entire Commonwealth of Virginia. The state is now divided into three local sections—Virginia, Virginia Blue Ridge, and Hampton Roads. In addition, a few counties in northern Virginia are part of the Washington Section, four counties in Southwest Virginia belong to the Northeast Tennessee Section, and there are some rural counties that are not part of any local section. The Virginia Blue Ridge Section was carved out of the Virginia Section in 1931. The Hampton Roads Section was formed some years later. The new Tidewater local section had 54 charter members (the Virginia Section had 301 at the time). **In what year was the Hampton Roads Section chartered?** The Hampton Roads Section was granted a charter by the ACS in 1944. An article in the Virginia Section Bulletin said that "This happy event, the second such in the history of the Mother section, was welcomed by all as evidencing the growth of chemistry in the Old Dominion. The offspring was a lusty infant with fifty-four charter members." The new Section replaced the Hampton Roads Chemists Club. The first Chairman of the Hampton Roads Section was Frank W. Wilder. Its first meeting was held at the Portsmouth Y.M.C.A. on November 9, 1944 when Dr. Roscoe H. Gerke spoke on "Rubber Properties."

New question: The Virginia Section received an award from the ACS at the Miami Beach national meeting for being the Outstanding Local Section in the medium-large category. Sheryl Baldwin received the award for the Section. Others in attendance at the awards ceremony included Allan Powell, Councilor; Oscar Rodig, Councilor; and Jerry Bass, Alternate Councilor. **What year was the award given to the Virginia Section?**

**CHEMISTRY DEPARTMENTS AT COLLEGES AND UNIVERSITIES
IN THE VIRGINIA SECTION**

<u>School/Location</u>	<u>Department Chair/ Program Coordinator</u>	<u>Phone/E-mail</u>
Bridgewater College Bridgewater, VA 22812	Dr. Joseph Crockett	(540) 828-5431 jcrocket @ bridgewater.edu
College of William & Mary Williamsburg, VA 23187-8795	Dr. Gary W. Rice	(757) 221-2540 gwrice @ wm.edu
Eastern Mennonite University Harrisonburg, VA 22802	Dr. Stephen G. Cessna	(540) 432-4403 cessnas @ emu.edu
Hampden-Sydney College Hampden-Sydney, VA 23943	Dr. C. William Anderson	(434) 223-6179 Wanderson @ hsc.edu
James Madison University Harrisonburg, VA 22801	Dr. Donna S. Amenta	(540) 568-6246 amentads @ jmu.edu
Longwood College Farmville, VA 23909	Dr. Melissa Rhoten	(434) 395-2636 rhotenmc @ longwood.edu
Mary Baldwin College Staunton, VA 24401	Dr. Vladimir Garkov	(540) 887-7102 vgarkov @ mbc.edu
Randolph-Macon College Ashland, VA 23005	Dr. Serge Schreiner	(804) 752-7206 sschrein @ rmc.edu
St. Paul's College Lawrenceville, VA 23868	Dr. Sunday A. Adesuyi	(434) 848-6484 sadesuyi @ saintpauls.edu
Shenandoah University Winchester, VA 22601	Dr. John Happ	(540) 665-4591 jhapp @ su.edu
University of Mary Washington Fredericksburg, VA 22401	Dr. Kelli Slunt	(540) 654-1406 kslunt @ umw.edu
University of Richmond Richmond, VA 23173	Dr. John Gupton	(804) 287-6498 jgupton @ richmond.edu
University of Virginia Charlottesville, VA 22901	Dr. Ian Harrison	(434) 924-3639 harrison @ virginia.edu
Virginia Commonwealth Univ. Richmond, VA 23284	Dr. Nicholas P. Farrell	(804) 828-1298 mpfarrel @ vcu.edu
Virginia State University Petersburg, VA 23806	Dr. Ralph Gatrone	(804) 524-5438 rgatrone @ vsu.edu
Virginia Union University Richmond, VA 23220	Dr. Dorothy Eseonu	(804) 257-5615 dneseonu @ vuu.edu

THE BULLETIN

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Bulletin Publisher - Dr. Will Lewis (804) 274-5869

CAN YOU IDENTIFY THIS PERSON?



The photograph is from the year 1944 when the subject was chair of the Virginia Section. Born in Morristown, Pennsylvania, the son of a Brigadier-General and a "Connecticut Yankee," he was a direct descendent of Thomas Jefferson. He graduated from Woodberry Forest School, then received a B.S. and an M.S. in Chemical Engineering from MIT. In 1938 he received a Ph.D. degree from the University of Virginia. He was employed by the Virginia-Carolina Chemical Corporation where he was active in improving the art of baking. He also made contributions to the field of detergents. In 1957 the Virginia Section presented him with its Distinguished Service Award.

The "Mystery persons" shown in the September Bulletin were Jerry Bass, Helmut Wakeham, and Bill Kuhn (left-to-right). Jerry and Bill were the Chairpersons of the 1991 SERMACS meeting that was held in Richmond. Helmut was the Meeting Chairman for the 1969 SERMACS meeting, also held in Richmond.

