

DCP Invited Speakers
March 2012 National Meeting
Feb. 27-Mar. 2, 2012 in Boston

Prepared by Donald G. Truhlar, Program Chair for the 2012 meeting

The Division of Chemical Physics will have six symposia at the March 2012 meeting:

Chemical Physics for New Energy

Density Functional Theory for Chemical Physics

Chemical Physics of the Environment

Impact of Ultrafast Lasers in Chemical Physics: Advances in Nonlinear Spectroscopies, Light Sources, and Applications

Chemical Physics of Clusters, Nanoparticles, and Nanoscale Materials

Symposium in honor of the recipient of the Earle K. Plyler Prize for Molecular Spectroscopy and Dynamics: Andrei Tokmakoff

The invited speakers are as follows:

	Invited Speaker	Tentative Talk Title
	Chemical Physics for New Energy Organizers: Bruce Garrett and Anders Nilsson	
1	Prof. Charles Campbell University of Washington Box 351700 Seattle WA 98195-1700 campbell@chem.washington.edu	Interfacial binding in catalytic and photovoltaic materials, and the energetics of elementary surface processes during catalytic fuels production and utilization
2	Prof. Emily Carter Princeton University Department of Mechanical and Aerospace Engineering D404A Engineering Quadrangle Princeton, NJ 08544 eac@princeton.edu	Transport in and chemistry on transition metal oxides for energy conversion

3	<p>Prof. Russell Hemley Carnegie Institution of Washington 5251 Broad Branch Road, NW Washington, DC 20015 rhemley@ciw.edu</p>	<p>Energy materials in extreme environments</p>
4	<p>Dr. Gregory Kimmel Pacific Northwest National Laboratory PO Box 999, MSIN: K8-88 Richland, WA 99352 gregory.kimmel@pnnl.gov</p>	<p>New photochemical pathways for oxygen on TiO₂(110)</p>
5	<p>Dr. Nenad Markovic Argonne National Laboratory Material Science 9700 S. Cass Avenue, Bldg. 223, A-225 Argonne, Illinois 60439 USA nmmarkovic@anl.gov</p>	<p>Energy conversion and fuel production from electrochemical interfaces</p>
6	<p>Prof. Horia Metiu University of California, Santa Barbara Department of Chemistry and Biochemistry Office: 4148A Chem Santa Barbara CA 93106-9510 metiu@chem.ucsb.edu</p>	<p>Alkane and CO₂ activation by modified oxide catalysts</p>
7	<p>Prof. Jens Norskov Stanford University Mail Code 5025 Stanford, CA 94305 norskov@stanford.edu</p>	<p>Understanding the link between surface electronic structure and reactivity</p>
8	<p>Prof. Richard Osgood Columbia University 1324 S. W. Mudd, Mail Code: 4712 500 West 120th Street New York, NY 10027 osgood@columbia.edu</p>	<p>Probing the nanointerface for nanoparticle-based solar energy conversion: Molecular dynamics on the Angstrom scale</p>
9	<p>Prof. Mark Ratner Northwestern University Department of Chemistry 2145 Sheridan Road Evanston, IL 60208-3113 ratner@chem.northwestern.edu</p>	<p>Molecular photovoltaics: Tricks from theory, from fission to gaps to traps</p>

10	<p>Dr. Eric Rohlfiing Chemical Sciences, Geosciences, and Biosciences Division Office of Basic Energy Sciences SC-22.1/Germantown Building U.S. Department of Energy 1000 Independence Avenue, SW Washington, D.C. 20585-1290 eric.rohlfiing@science.doe.gov</p>	<p>Facing our energy challenges in a new era of science</p>
11	<p>Dr. Kevin Rosso Pacific Northwest National Laboratory PO Box 999, MSIN: K8-96 Richland, WA 99352 Kevin.Rosso@pnnl.gov</p>	<p>Coupled polaronic and ion transport in nanocrystalline metal oxide electrodes</p>
12	<p>Prof. George C. Schatz Northwestern University Department of Chemistry 2145 Sheridan Road, Evanston, IL 60208-3113 schatz@chem.northwestern.edu</p>	<p>Theories of plasmon enhanced optical processes important in solar energy</p>
13	<p>Prof. Gregory Voth University of Chicago 5735 S. Ellis Ave., SCL 231, Chicago, IL 60637 gavoth@uchicago.edu</p>	<p>Multiscale simulation of electrochemical phenomena: Fuel cells and batteries</p>
14	<p>Prof. Peidong Yang University of California, Berkeley B68 Hildebrand Departments of Chemistry and Materials Science and Engineering Berkeley, CA 94720 p_yang@uclink.berkeley.edu</p>	<p>Semiconductor nanostructures for artificial photosynthesis</p>
	<p>Density Functional Theory for Chemical Physics Organizers: Kieron Burke and Neepa Mairtra</p>	
1	<p>Valentino Cooper coopervr@ornl.gov Materials Science and Technology Division Materials Theory Group P.O. Box 2008 MS-6114 Oak Ridge National Laboratory Oak Ridge, TN 37831-6114</p>	<p>Understanding the role of London dispersion forces in molecular surface processes</p>

2	<p>Hardy Gross hardy@mpi-halle.mpg.de Max-Planck-Institut für Mikrostrukturphysik Weinberg 2 D - 06120 Halle Germany</p>	<p>Derivative discontinuity of the xc kernel of TDDFT and the description of excitons and charge-transfer excitations</p>
3	<p>Erin Johnson ejohnson29@ucmerced.edu School of Natural Sciences University of California, Merced Merced, CA, 95343</p>	<p>Real-space DFT models for strong correlation</p>
4	<p>Miguel Marques marques@tddft.org Lab. de Physique de la Matière Condensée et Nanostructures Université Lyon 1 et CNRS Bâtiment Brillouin, Domaine scientifique de la DOUA 69622 Villeurbanne Cedex France</p>	<p>New density functionals and old problems</p>
5	<p>Tom Miller tfm@caltech.edu Division of Chemistry and Chemical Engineering California Institute of Technology 1200 E. California Boulevard Mail Code 164-30 CA 91125</p>	<p>Exactly embedded density functional theory methods for condensed phase reactions</p>
6	<p>John Perdew perdew@tulane.edu Department of Physics, Engineering Physics, and Astronomy School of Science and Engineering Tulane University New Orleans, LA 70118, USA</p>	<p>Improved semilocal and nonlocal density functionals for atoms, molecules, and solids</p>
7	<p>Angel Rubio angel.rubio@ehu.es NanoBio Spectroscopy Group and ETSF Scientific Development Centre Department of Materials Science, Faculty of Chemistry University of the Basque Country UPV/EHU Centro Joxe Mari Korta, Avenida de Tolosa, 72, E-20018 Donostia-San Sebastian, Spain</p>	<p>TDDFT for nonlinear phenomena of light-matter interactions</p>

8	<p>Charles Stafford stafford@physics.arizona.edu University of Arizona 1118 E. 4th Street Tucson, AZ 85721, USA</p>	<p>On the derivative discontinuity in molecular junctions</p>
9	<p>Carsten Ullrich ullrichc@missouri.edu Department of Physics & Astronomy University of Missouri Columbia, MO 65211</p>	<p>Watching excitons move: the time-dependent transition density matrix</p>
10	<p>Troy van Voorhis tvan@mit.edu MIT Department of Chemistry 77 Massachusetts Ave. Cambridge, MA 02139</p>	<p>Nonlocal density functionals for van der Waals interactions</p>
11	<p>Adam Wasserman awasser@purdue.edu Department of Chemistry Purdue University 560 Oval Drive West Lafayette, IN - 47907</p>	<p>Partition Density Functional Theory</p>
12	<p>Weitao Yang Weitao.Yang@duke.edu Department of Chemistry Duke University 124 Science Dr. Box 90354 Durham, NC 27708-0354</p>	<p>Progress in the fractional perspectives of DFT</p>
13	<p>Donald G. Truhlar University of Minnesota 207 Pleasant Street SE 139 Smith Hall Minneapolis, MN 55455-0431 Truhlar@umn.edu</p>	<p>SOGGA11, SOGGA11-X, M11, and M11-DL: Density functionals satisfying the second order constraint and having broad applicability in chemical physics</p>
14	<p>E. Miles Stoudenmire 310N Rowland Hall Department of Physics University of California, Irvine Irvine, CA 92697-4675 miles.stoudenmire@gmail.com</p>	<p>Exact DFT Calculations with the Density Matrix Renormalization Group (DMRG)</p>

	<p>Chemical Physics of the Environment Organizers: Donald Baer and J. Ilja Siepmann</p>	
1	<p>William F. Schneider University of Notre Dame 123b Cushing Hall 182 Fitzpatrick Hall Notre Dame, IN 46556 574-631-8754 wschneider@nd.edu</p>	<p>Metal oxides for environmental NO_x catalysis</p>
2	<p>Dr. David Shuh Lawrence Berkeley National Laboratory MS: 70A-1150 One Cyclotron Rd. Berkeley, CA 94720 510-486-6937 dkshuh@lbl.gov</p>	<p>Assessing Actinide-Oxygen Covalency by K-edge X-ray Absorption Spectroscopy</p>
3	<p>Prof. Edward J. Maginn Dept. of Chemical and Biomolecular Engineering University of Notre Dame Notre Dame, IN 46556 574-631-5687 ed@nd.edu</p>	<p>Using molecular simulation to develop new ionic liquids for energy and environmental applications</p>
4	<p>Dr. James E. Hutchinson University of Oregon 1253 University of Oregon Eugene, OR 97403 541-346-4228 hutch@uoregon.edu</p>	<p>Physical study of nanoparticle transformations to guide design of greener products and processes</p>
5	<p>Hanna Vehkamäki Dept. of Physics PO Box 64 (Gustaf Hällströmin katu 2a) FI-00014 University of Helsinki Finland +358 (0)50 4154747 Hanna.vehkamaki@helsinki.fi</p>	<p>Uncovering the formation mechanism of atmospheric nanoparticles</p>
6	<p>Vicki H. Grassian University of Iowa Dept. of Chemistry 305 Chemistry Bldg Iowa City, IA 52242 319-335-1392</p>	<p>Optical Properties and Heterogeneous Photochemistry of Mineral Dust Aerosol</p>

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7	Michael F. Hochella, Jr. Virginia Tech 4044 Derring Hall Blacksburg, VA 24061 540-231-6227 hochella@vt.edu	Nanominerals, Mineral Nanoparticles, and Earth Processes: Details on how nanoparticles Work in the Environment
8	Dr. John H. Weare University of California San Diego Dept. Chemistry & Biochemistry 9500 Gilman Dr. #0340 La Jolla, CA 92093 858-534-7244 jweare@ucsd.edu	1st principle simulations of ions in water solutions: Bond structure and chemistry in the hydration shells of highly charged ions
9	Heather C. Allen The Ohio State University Dept. of Chemistry & Biochemistry 100 W. 18th Ave. Columbus, OH 43210 614-292-4707 allen@chemistry.ohio-state.edu	Organization at the Air-Aqueous Interface by Phase-Sensitive Sum Frequency Spectroscopy
10	Dermot Diamond Chemical Sciences Dublin City University Dublin 9, Ireland +353-1-7005404 Dermot.diamond@dcu.ie	Autonomous Chemical Sensor Networks for Distributed Environmental Monitoring - Can the dream become Reality?
11	Dr. Omowunmi A. Sadik SUNY Binghamton Dept. of Chemistry PO Box 6000 Binghamton, NY 13902 607-777-4132 osadik@binghamton.edu	Sensors as probes for the environmental dynamics of nanostructured materials

	<p>Impact of Ultrafast Lasers in Chemical Physics: Advances in Nonlinear Spectroscopies, Light Sources, and Applications</p> <p>Organizers: Amber Krummel and Nancy Levinger</p>	
1	<p>Amy Mullin 0107 Chemistry Bldg. Dept. of Chemistry & Biochemistry University of Maryland College Park, MD 20742 301-405-6569 mullin@umd.edu</p>	High-Resolution Transient Optical Probing
2	<p>Thomas Elsaesser Max-Born-Institute Max-Born-Str. 2A 12489 Berlin, Germany elsasser@mbi-berlin.de</p>	Ultrafast molecular processes mapped by femtosecond x-ray diffraction"
3	<p>Greg Engel University of Chicago 929 East 57th St. Chicago, IL 60637 gsengel@uchicago.edu</p>	Two dimensional electronic spectroscopy of coherent energy transfer processes."
4	<p>Shaul Mukamel Department of Chemistry 516 Rowland Hall Suite RH434 University of California Irvine, CA 92697-2025 smukamel@uci.edu</p>	Probing amyloid fibrils and Light Harvesting complexes by multidimensional optical spectroscopy of excitons
5	<p>Margaret Murnane JILA, University of Colorado at Boulder Boulder, CO 80309-0440 Margaret.Murnane@colorado.edu</p>	Capturing the Coupled Dynamics of Electrons, Atoms and Spins in Molecules and Materials using Ultrafast X-Rays
6	<p>Keith Nelson MIT Room 6-235 Department of Chemistry 77 Massachusetts Avenue Cambridge, MA 02139 kanelson@mit.edu</p>	Control over coherent light fields enables multidimensional coherent spectroscopy and multispectral coherent control"

7	Jennifer Ogilvie Department of Physics/Biophysics University of Michigan 450 Church St. Ann Arbor, MI 48109 jogilvie@umich.edu	Probing photosynthetic structure and function using multidimensional spectroscopy
8	Gregory Scholes Department of Chemistry University of Toronto 80 St. George Street Toronto, Ontario, M5S 3H6 greg.scholes@utoronto.ca	Quantum mechanical light harvesting mechanisms in photosynthesis
9	Martin Zanni Department of Chemistry 1101 University Ave., Room 8361 Madison, WI 53706 zanni@chem.wisc.edu	New Technologies for mid-IR pulse shaping and its application to 2D IR spectroscopy
10	Kelly Gaffney Assistant Professor, PULSE Institute for Ultrafast Energy Science, SLAC National Accelerator Laboratory 2575 Sand Hill Rd, Mail Stop 69, Menlo Park, CA, 94025-7015 Tel : (650) 926-2382 Fax: (650) 926-4100 kgaffney@slac.stanford.edu	Ultrafast X-Ray Laser Studies of Chemical Dynamics
	Chemical Physics of Clusters, Nanoparticles, and Nanoscale Materials Organizers: S. N. Khanna and Gabor Somorjai	
1	Richard P. Van Duyne Northwestern University Chemistry Department 2145 Sheridan Rd. Evanston IL 60208-3113 Phone: 847-491-3516 vanduyne@northwestern.edu	New Directions in Plasmonics: Pushing the Space-Time Limit
2	Mark R. Pederson PhD Chemical Sciences, Biosciences, and Geosciences Division Office of Basic Energy Sciences US Department of Energy 19901 Germantown Road, Room E-433 Germantown, MD 20874-1920 US	DFT for Field-Dependent Control of Nanomagnetic Clusters and Molecules

	Phone: (301) 903-9956, Fax: (301) 903-0271 mark.pederson@science.doe.gov	
3	Dr. Everett E. Carpenter Associate Professor of Inorganic and Materials Chemistry Affiliate Professor of Chemical and Life Science Engineering 1001 West Main Street Department of Chemistry Virginia Commonwealth University Richmond VA, 23284 804-828-7508 (voice) 804-828-8599 (fax) ecarpenter2@vcu.edu www.nano.vcu.edu ecarpenter2@vcu.edu	Novel Permanent Magnets without Rare-earth Elements
4	Paul Alivisatos Department of Materials Science and Engineering D43 Hildebrand University of California, Berkeley Berkeley, CA 94720 tel:(510)643-7371 fax:(510)642-6911 alivis@berkeley.edu	Direct imaging of colloidal nanoparticle growth, structure, and assembly in a transmission electron microscope
5	Francisco Zaera 501 Big Springs Road, Chemical Sciences #146 Riverside, CA 92521 Tel: (951) 827-5498 (Office) Tel: (951) 827-5736 (Lab) Fax: (951) 827-3962 (Direct) Fax: (951) 827-4713 Department zaera@ucr.edu	Design of nanocatalysts for improved selectivity and stability
6	Charles M. Lieber Department of Chemistry and Chemical Biology Harvard University 12 Oxford Street Cambridge, MA 02138 cml@cmliris.harvard.edu	Semiconductor Nanowires
7	Scott L. Anderson Chemistry Dept 315 S. 1400 E., Rm 2020 Salt Lake City, UT 84112	Size-Dependent Activity, Stability, and Adsorbate Binding of Model Size- Selected Catalysts

	(801)585-7289 anderson@chem.utah.edu	
8	A. Welford Castleman, Jr. Departments of Chemistry and Physics 104 Chemistry Building Penn State University University Park, PA 16802 (814) 865-7242 - Office Phone (814) 865-5235 - Fax awc@psu.edu	Cluster Structure and Reactions: Gaining insight into catalytic processes
9	Donald A. Tomalia The National Dendrimer & Nanotechnology Center Central Michigan University 1200 N. Fancher Mt. Pleasant, Michigan 48858 USA Phone 989-317-3737 donald.tomalia@nanosynthons.com	In Quest of a Systematic Framework for Unifying and Defining Nanoscience
	Plyler Prize Symposium Organizer: Donald G. Truhlar Session chair: Birgitta Whaley, Division Chair	
1	Andrei Tokmakoff Department of Chemistry, Room 6-213 77 Massachusetts Avenue Cambridge, MA 02139 (617) 253-4503 tokmakof@mit.edu	Prize Lecture
2	James Skinner Department of Chemistry University of Wisconsin 1101 University Avenue Madison WI 53706 608-262-0481 skinner@chem.wisc.edu	Modern vibrational spectroscopy of water in its condensed phases
3	David Jonas Department of Chemistry and Biochemistry Co-Director, Center for Revolutionary Solar Photoconversion University of Colorado Boulder, CO 80309 (303) 492-3818 jonasd@stripe.Colorado.EDU	Two-Dimensional Fourier Transform Electronic Spectroscopy