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Mesoscale Chemistry

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Speaker Biographies

Andrew Borovik, Ph.D., University of California-Irvine, Irvine, California

Andrew Borovik, Ph.D., was born and raised in Chicago, Illinois and obtained his B.S. degree in Chemistry from Humboldt State University, in Arcata, California in 1981. In 1986, he received his Ph.D. from the University of North Carolina-Chapel Hill, under Professor Tom Sorrell. Dr. Borovik has held postdoctoral positions with Larry Que at the University of Minnesota as an NIH fellow from 1986-1988 and Ken Raymond at the University of California-Berkeley from 1990-1992. He has been on the faculty at Ithaca College, Kansas State University, the University of Kansas, and the University of California-Irvine, where he is currently a professor.
His research group has been developing new approaches in molecular design to prepare synthetic constructs that emulate the properties of protein active sites. Protein active sites have unique architectural features that control the immediate environment surrounding metal ions (microenvironment). These features, in turn, are instrumental in controlling protein activity, much of which has not yet been achieved in synthetic systems. Non-covalent interactions, particularly hydrogen bonds (H-bonds) have been implicated as key regulators of microenvironmental properties. However, little is known about how H-bonds are able to influence metal-mediated processes. By establishing non-covalent interactions that promote the activation of small molecules, his group can control the secondary coordination sphere of metal complexes.

Jim De Yoreo, Ph.D., Pacific Northwest National Laboratory (PNNL), Richland, Washington

Jim De Yoreo is Chief Scientist for Materials Synthesis and Simulation Across Scales at PNNL and an Affiliate Professor of Materials Science and Engineering at the University of Washington. He received his Ph.D. in Physics from Cornell University in 1985. Following post-doctoral work at Princeton University, he became a member of the technical staff at Lawrence Livermore National Laboratory in 1989, where he held numerous positions including Director of the Biosecurity and Nanosciences Laboratory, and Deputy Director of the Laboratory Science and Technology Office. He joined Lawrence Berkeley National Laboratory in 2007 where he served as Deputy and Interim Director of the Molecular Foundry. DeYoreo is a member of the MRS, APS, ACS and the AACG. He is an Editor for Bioinspired Materials, Associate Editor in Chief for Frontiers of Materials Science, and a member of the Executive Committee of the International Organization for Crystal Growth (IOCG). He has served as President and Board Member of the Materials Research Society and on committees for the National Academy of

Sciences, the Department of Energy, and the US Congress. De Yoreo's research has spanned a wide range of materials-related disciplines, focusing most recently on *in situ* AFM and TEM investigations of interactions, assembly, and crystallization in biomolecular and biomineral systems. De Yoreo has authored, co-authored, or edited over 195 publications and patents. He is a recipient of the IOCG's Laudise Prize, the AACG Crystal Growth Award, an R&D 100 Award, and the LLNL Science and Technology Award, and is a Fellow of the APS and the MRS.

John Spencer Evans, D.D.S., Ph.D., New York University, New York, New York

Dr. Evans received his B.S. degree at Northwestern University and his D.D.S. degree at the University of Illinois in 1982. After completing residency fellowships at Northwestern University Medical Center and the University of Southern California Medical Center, he obtained his PhD in Chemistry at California Institute of Technology in 1993. He is currently a Professor at the Center for Skeletal Sciences, New York University, and his research emphasis is on protein-mediated biomineralization phenomena.

Alexander C. Gagnon, Ph.D., University of Washington, Seattle, Washington

Alexander C. Gagnon received his B.S. and B.A. degrees from University of California, Berkeley in 2002. Remaining on the west coast, he completed his doctorate studies under Professor Jess Adkins and Douglas Rees at California Institute of Technology with a thesis entitled, "Geochemical Mechanisms of Biomineralization from Analysis of Deep=Sea and Laboratory Cultured Corals" in 2010. From 2010-2013 Dr. Gagnon held a postdoctoral fellowship at the Lawrence Berkeley National Lab with Donalad De Paolo and James DeYoreo. Gagnon was appointed Assistant Professor in the School of Oceanography at University of Washington in 2013, where he is currently.

Pupa Gilbert. Ph.D., University of Wisconsin-Madison, Madison, Wisconsin

Trained in Physics at the First University of Rome La Sapienza with Filippo Conti (Chemistry, Physical Chemistry) and Tiziana Parasassi (Biology, Biochemistry), Pupa Gilbert has 30 years of experience in the fascinating field of Biophysics. She has been a staff scientist at the Italian CNR in 1988-1999, and at the Swiss Institute of Technology in 1994-1998, until she joined the Physics Department at University of Wisconsin-Madison in 1999 as a full professor. She won many awards in Italy, the US, and internationally. She served as Scientific Director of the Synchrotron Radiation Center in 2002-2006, on the Scientific Advisory Committee of the Canadian Light Source 2004-2009, and as Chair of the Division of Biological Physics of the American Physical Society (APS) in 2010-2014. She is a Fellow of the APS and of the Radcliffe Institute for Advance Study at Harvard University.

Sharon Glotzer, Ph.D., University of Michigan, Ann Arbor, Michigan

Dr. Glotzer is the Stuart W. Churchill Collegiate Professor of Chemical Engineering, and Professor of Materials Science and Engineering, Physics, Applied Physics, and Macromolecular Science and Engineering at the University of Michigan in Ann Arbor. She is member of the

National Academy of Sciences, and a fellow of the American Academy of Arts and Sciences, the American Physical Society, and the American Association for the Advancement of Science. She received the B.S. degree from the University of California, Los Angeles, and the Ph.D. degree from Boston University, both in physics. Prior to joining the University of Michigan in 2001 she worked for eight years in the Materials Science & Engineering Laboratory at the National Institute of Standards and Technology as co-founder and Director of the NIST Center for Theoretical and Computational Materials Science. Glotzer's research on computational assembly science and engineering aims toward predictive materials design of colloidal and soft matter, with current emphasis on shape, packing, and assembly pathways. She has nearly 200 refereed publications and has presented over 300 plenary, keynote and invited talks around the world. Glotzer was the recipient of the Charles M.A. Stine Award in Materials Science and Engineering from the American Institute of Chemical Engineers, holds a National Security Science and Engineering Faculty Fellowship from the Office of the Secretary of Defense, and was named a 2012 Simons Investigator.

Cynthia Jenks, Ph.D., The Ames Laboratory, Ames, Iowa

Dr. Cynthia Jenks is the Assistant Director for Scientific Planning and the Division Director of Chemical and Biological Science at the Ames Laboratory. She received her B.S. in Chemical Engineering in 1986 from the University of California, Los Angeles. She received a M.S. degree in Chemical Engineering in 1988 and a Ph.D. in Chemistry from Columbia University in 1992. She did her postdoctoral work at Iowa State University and the U.S. Department of Energy's Ames Laboratory. She joined the scientific staff of the Ames Laboratory in 1995. Her research interests are in the areas of surface structure and reactivity, surface structure-property relationships, catalysis, and thin film growth. She is a Fellow of the American Association for the Advancement of Science.

Erwin London, Ph.D., Stony Brook University, Stony Brook, New York

Dr. London received his B.A. at Queens College of the City University of New York in 1974 and completed his Ph.D. at Cornell University in 1980. After completing his Ph.D., London accepted a postdoctoral fellowship at Massachusetts Institute of Technology from 1980-1982. Since then, he has been a part of the faculty at Stony Brook University. He is currently professor in the Department of Biochemistry and Cell Biology and has a joint appointment in the Department of Chemistry.

His research group studies biomembrane protein structure and function and biomembrane lipid and protein organization by combining spectroscopic methods, such as fluorescence, with chemical, biochemical, immunochemical and molecular biological approaches. Recent studies have concentrated upon understanding the organization of biomembranes into domains with distinct lipid and protein compositions. Biomembrane lipid segregation into domains of high structural order (lipid rafts) and lower structural order (liquid disordered domains) has become an important focus of cell membrane studies. Lab studies aim at defining the principles that underlie domain formation and developing methods to detect such domains in cells. To aid in this, the lab has developed a model biomembrane vesicle system that for the first time efficiently

reproduces the lipid asymmetry (difference in lipid chemical composition) in the inner (cytoplasmic) and outer (exofacial) monolayers found in the lipid bilayers of many cell membranes.

Yi Lu, Ph.D., University of Illinois, Urbana-Champaign, Urbana, Illinois

Dr. Yi Lu received his B.S. degree from Peking University in 1986, and Ph.D. degree from University of California at Los Angeles in 1992 under Professor Joan S. Valentine. After two years of postdoctoral research in Professor Harry B. Gray group at the California Institute of Technology, Dr. Lu started his own independent career in the Department of Chemistry at the University of Illinois at Urbana Champaign in 1994. He is now Jay and Ann Schenck Professor of Chemistry in the Departments of Chemistry, Biochemistry, Bioengineering and Materials Science and Engineering. He is also a member of the Center for Biophysics and Computational Biology and Beckman Institute for Advanced Science and Technology. His research interests lie at the interface between chemistry and biology. His group is developing new chemical approaches to provide deeper insight into biological systems. At the same time, they take advantage of recently developed biological tools to advance many areas in chemistry. Specific areas of current interests include a) design and engineering of functional metalloproteins as environmentally benign catalysis in renewable energy generation and pharmaceuticals; b) Fundamental understanding of DNAzymes and their applications in environmental monitoring, medical diagnostics, and targeted drug delivery; and c) Employing principles from biology for directed assembly of nanomaterials with controlled morphologies and its applications in imaging and medicine.

Andrew Madden, Ph.D., University of Oklahoma, Norman, Oklahoma

Dr. Andrew Elwood Madden is an associate professor in the School of Geology and Geophysics at University of Oklahoma where he co-directs the Physical and Environmental Geochemistry Laboratory and directs the powder X-ray diffraction laboratory. His B.S. degree in geology from Michigan State University was followed by a Ph.D. in geochemistry from Virginia Tech while holding an NSF Graduate Research Fellowship and postdoctoral research at Oak Ridge National Laboratory. In recent years, his research on nanoparticulate minerals ranged from fundamental studies comparing the size-dependent reactivity of nanoparticulate minerals in the lab and field, the formation of nanoparticulate phases of radionuclides and metals for groundwater remediation, the frictional properties of nanoparticulate rock gouge that control the behavior of fault zones in earthquakes, to nanodiamonds in natural sediments as possible indicators of an impact event at the Younger Dryas boundary, and analog studies of nanoparticulate iron oxide minerals that constrain the history of water on Mars. He also teaches courses such as Physical Geology, Environmental Geology, Minerals and the Environment, and Clay Mineralogy.

William Noid, Ph.D., Pennsylvania State University, University Park, Pennsylvania

William Noid received his B.S. degree from the University of Tennessee in 2000. He moved to Ithaca to complete his Ph.D. at Cornell University in 2005 for research in quantum-classical

theories of nonlinear spectroscopy. He was an NIH NRSA postdoctoral fellow at the University of Utah, where he worked on multiscale modeling theories with Prof. G.A. Voth. He started as an assistant professor at Penn State in 2007 and was promoted to associate professor in 2013. His research at Penn State addresses theories for multiscale modeling, glycoprotein biophysics, and intrinsically disordered proteins. This work has been recognized by an ACS Hewlett Packard Outstanding Junior Faculty Award, an Alfred P Sloan Foundation fellowship, a Camille Dreyfus Teacher-Scholar award, and an NSF Career award.

Klaus Schulten, Ph.D., University of Illinois at Urbana-Champaign, Urbana, Illinois

Klaus Schulten holds a Diplom degree in physics from the University of Muenster, Germany (1969), and a PhD in chemical physics from Harvard University (1974). He was junior group leader at the Max-Planck-Institut for Biophysical Chemistry from 1974 to 1980, and professor of theoretical physics at the Technical University of Munich from 1980 to 1988. Schulten came to the University of Illinois in 1988, and in 1989 joined the Beckman Institute and founded the Theoretical and Computational Biophysics Group, which operates the NIH Center for Macromolecular Modeling and Bioinformatics. Since 2008 he is co-director of the NSF-funded Center for the Physics of Living Cells. Schulten's awards and honors include: Blue Waters Professorship, National Center for Supercomputing Applications (2014); Professorship, University of Illinois Center for Advanced Study (2013); Distinguished Service Award, Biophysical Society (2013); IEEE Computer Society Sidney Fernbach Award (2012); Fellow of the Biophysical Society (2012); Award in Computational Biology (2008); Humboldt Award of the German Humboldt Foundation (2004); University of Illinois Scholar (1996); Fellow of the American Physical Society (1993); Nernst Prize of the Physical Chemistry Society of Germany (1981).

Wendy Shaw, Ph.D., Pacific Northwest National Laboratory (PNNL), Richland, Washington

Dr. Wendy Shaw received her B.A. in Chemistry from Whitman College in Walla Walla, Washington and obtained her Ph.D. at the University of Washington in 2000. Soon after, she landed a position at Pacific Northwest National Laboratory in Washington State, where her research interests are in the areas of catalysis and biomineralization. In catalysis, she is interested in understanding the contribution of the outer coordination sphere to organometallic catalysis by incorporating enzymatic features of the protein scaffold into homogeneous catalysts. The features of the outer coordination sphere being investigated include dynamics, the local environment around the active site and the function of proton channels. Dynamics are being studied with novel stimuli controlled ligands for catalyst control, development and recovery. The roel of the environment around the active site and the role of proton channels are being investigated with a combined computational and experimental approach building around nickel based hydrogen production/oxidation catalysts which mimic hydrogenase enzymes.

Her interests in biomineralization processes include developing a fundamental understanding of protein-surface interfaces and biomineralization processes using solid state NMR dipolar recoupling techniques, neutron reflectivity and physical chemistry methods. Specifically,

elucidating the protein structure, protein orientation and nucleation and growth mechanisms of naturally occurring biominerals. Broader implications include understanding non-natural systems such as protein-polymer interactions, coatings, and tissue engineering.

She has received several honorable awards including the Graduate Fellowship, Associated Western Universities from 1996-2000, Outstanding Performance Awards, PNNL, the DOE Early Career Program Grant, 2010, and was selected to attend the U.S.-Indonesia Symposium in 2011.

Peter Stair, Ph.D., Northwestern University, Evanston, Illinois

Peter C. Stair is the John G. Searle Professor of Chemistry and Chair of the Department of Chemistry at Northwestern University. He received a B.S. in Chemistry from Stanford University in 1972 and a Ph.D. from University of California, Berkeley in 1977 under the supervision of Gabor Somorjai. He has been on the faculty at Northwestern University since 1977. From 1997 to 2012 he was Director of the Northwestern University Center for Catalysis and Surface Science. He is Director of the Institute for Catalysis in Energy Processes, a Senior Scientist in the Chemical Sciences and Engineering Division at Argonne National Laboratory, and Deputy Director of the Energy Frontier Research Center: Institute for Atom-efficient Chemical Transformations. His research interests are in the synthesis, characterization, and physical properties of heterogeneous catalysts. He has worked in surface science and in-situ Raman spectroscopy. His goal is to develop fundamental understanding in catalysis science that leads to advances in industrial chemistry and energy technology. He is a past recipient of the Alexander von Humboldt Senior Scientist Award and recipient of the 2010 ACS George Olah Award in Hydrocarbon or Petroleum Chemistry.

Gregory Voth, Ph.D., University of Chicago, Chicago, Illinois

Dr.Voth is the Haig P. Papazian Distinguished Service Professor of Chemistry at The University of Chicago. He is also a Professor of the James Franck Institute and the Institute for Biophysical Dynamics, as well as a Senior Fellow of the Computation Institute. He received a Ph.D. in Theoretical Chemistry from the California Institute of Technology in 1987 and was an IBM Postdoctoral Fellow at the University of California, Berkeley from 1987-89. He is the author or co-author of approximately 425 peer-reviewed scientific articles, with an h-index of 78 and more than 22,000 citations. Voth is a Fellow of the American Chemical Society, American Physical Society, The Biophysical Society, and the American Association for the Advancement of Science. He has received a number of awards and other forms of recognition for his work, including most recently the American Chemical Society Division of Physical Chemistry Award in Theoretical Chemistry and Election to the International Academy of Quantum Molecular Science, both in 2013. He has proudly mentored more than 160 postdoctoral fellows and graduate students.

Professor Voth is a leader in the development and application of theoretical and computational methods to study problems involving the structure and dynamics of complex condensed phase systems, including proteins, membranes, liquids, and materials. He has pioneered a method known as “multiscale coarse graining” in which the resolution of the molecular-scale entities is

reduced into simpler structures, but key information on their interactions is accurately retained (or renormalized) so the resulting computer simulation can accurately and efficiently predict the properties of large assemblies of complex molecules such as lipids and proteins. This method is multiscale, meaning it describes complex condensed phase and biomolecular systems from the molecular scale to the mesoscale and ultimately to the macroscopic scale. Professor Voth's other research interests include the study of charge transport (protons and electrons) in water and biomolecules – a fundamental process in living organisms and other systems that has been poorly understood because of its complexity. He also studies the exotic behavior of room-temperature ionic liquids and other complex materials such a nanoparticle self-assembly, polymer electrolyte membranes for fuel cells, and electrode-electrolyte interfaces in energy storage devices. In the earlier part of his career, Professor Voth extensively developed and applied new methods to study quantum and electron transfer dynamics in condensed phase systems. Much of this work was based on the Feynman path integral description of quantum mechanics.

Aaron Wheeler, Ph.D., University of Toronto, Toronto, Canada

Dr. Wheeler completed his Ph.D. in Chemistry in 2003, working with Dick Zare at Stanford University. After graduating, Aaron spent two years as an NIH postdoctoral fellow at UCLA. Since 2005, Aaron has been the Canada Research Chair of Bioanalytical Chemistry at the University of Toronto, with a primary appointment in the Chemistry Department and cross-appointments at the Institute for Biomaterials and Bioengineering and the Banting and Best Department of Medical Research. Wheeler has been recognized internationally with a number of awards, including the Merck GmbH H.E.M. Prize and the American Chemical Society Arthur F. Findeis Award, and he is an Associate Editor of Lab on a Chip.

Benjamin Wilhite, Ph.D., Texas A&M University, College Station, Texas

Dr. Wilhite completed his doctoral research at Notre Dame. His focus included emphasizing reactor design and multiphase flow. From there, he moved to Boston, Massachusetts to complete a postdoctoral fellowship at M.I.T. where he focused upon catalytic micro reactors and micro membranes for energy applications. He began his academic career at the University of Connecticut from 2005-2010 and is currently a professor at Texas A&M University. His work centers on understanding interplay between transport phenomena, materials science and catalysis for designing membranes and micro reactors for natural gas processing.

Todd Yeates, Ph.D., University of California, Los Angeles, Los Angeles, California

Yeates earned his Bachelor's degree at UCLA in 1983. He stayed on at UCLA and earned his PhD in 1988 while doing research under the direction of Prof. Douglas Rees. There he helped determine the crystal structure of the bacterial photosynthetic reaction center as part of a team racing to determine the first crystal structures of membrane proteins. He then moved to The Scripps Research Institute to do his postdoctoral research on the structure of poliovirus with Prof. James Hogle. Yeates returned to UCLA in 1990 to join the Faculty in the Department of Chemistry and Biochemistry. His interdisciplinary research, combining molecular biology with computing and mathematics, has focused on structural, computational, and synthetic biology.

Past research findings in the Yeates lab include: an explanation for why proteins crystallize in certain favored arrangements, with implications for the development of 'racemic macromolecular crystallography'; the development of equations for detecting disorder in X-ray diffraction data from protein crystals; the discovery that certain thermophilic microbes are rich in intracellular disulfide bonds; development of comparative genomics methods; and the discovery of novel topological features such as links and slipknots, with implications for protein folding landscapes.

Recent work has focused on giant protein assemblies, both natural and designed. In the area of giant natural protein assemblies, Yeates' group has pioneered the structural biology of the carboxysome and related bacterial microcompartments. These are primitive metabolic organelles in many bacteria, wherein a protein shell (reminiscent of a viral capsid) encloses a series of enzymes in order to sequester a sensitive pathway within the bacterial cell. In the area of designed protein assemblies, Yeates' group has laid out symmetry-based strategies for engineering novel protein molecules to self-assemble into precisely defined symmetric nanocages and materials, and has demonstrated their successful application to creating cubic assemblies on the 15 to 20 nm scale. Yeates is a member of the Molecular Biology Institute, the California Nanosystems Institute, the UCLA-DOE Institute of Genomics and Proteomics, and a Fellow of the American Association for the Advancement of Science.