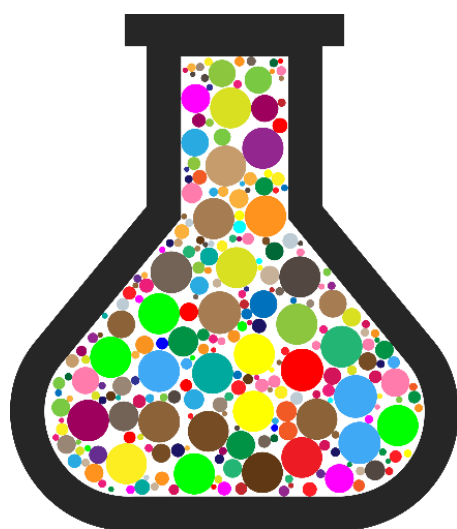


**The Department of Chemistry
Stony Brook University**

Presents

The 20th Annual

CHEMISTRY RESEARCH DAY



October 4, 2019



Stony Brook University
College of Arts and Sciences

CHEMISTRY RESEARCH DAY

PROGRAM

11:00 am – 12:30 pm	Poster Session I – Even-Numbered Posters Student Activities Center Ballroom A
12:30 pm – 1:30 pm	Participant Luncheon Student Activities Center Ballroom B
1:30 pm – 3:00 pm	Poster Session II – Odd-Numbered Posters Student Activities Center Ballroom A
3:00 pm – 3:15 pm	Reception Student Activities Center Why Lobby
3:15 pm – 4:45 pm	Keynote Lecture Student Activities Center Auditorium Introduction: Ilana Heckler Speaker: Professor Esther S. Takeuchi Title: From Medical Applications to the Environment: The Important Role of Energy Storage
5:00 pm – 7:00 pm	Chemistry Department Celebration! Chemistry Building Lobby

NO.	PRESENTERS	AUTHORS	TITLE
1	Alyson Abraham	Alyson Abraham, Jianping Huang, Mikaela R. Dunkin, Bingjie Zhang, Chavis A. Stackhouse, Paul F. Smith, Kenneth J. Takeuchi, Amy C. Marschilok, Esther S. Takeuchi	Self-Forming Li/I ₂ -Based Rechargeable Solid State Battery: Demonstration, Electrochemistry, and Interface Effects
2	Shin Hye (Grace) Ahn	Shin Hye Ahn, Brett Vaughn, Eszter Boros	Site-Specific Antibody Conjugation of Cleavable Metal Chelators for Nuclear Imaging and Therapy
3	Noel Amaro	Noel A. Amaro, Dipankar Sahoo, Jaehoon Jang, Francisco I. Caban, Salvatore J. Bracco, Jessica L. Humann, Manoj Kumar, Jonathan G. Rudick	Liquid Crystalline Dendrimers Prepared via the Passerini Three-Component Reaction
4	Ashwin Ambi	Ashwin Ambi, Tiffany W. Victor, Randy J. Smith, Feng Xu, Steven O. Smith, William Van Nostrand, Lisa Miller	Determining the Copper Levels in Amyloid Aggregates of Alzheimer's Disease Using X-ray Fluorescence Microscopy
5	Monaf Awwa	Monaf Awwa, Jinwoo Kim, Diane M. Bogdan, Matthew W. Elmes, Su Yan, Joyce Che, Garam Lee, Dale G. Deutsch, Robert Rizzo, Martin Kaczocha, Iwao Ojima	Biological and Computational Assessment of (-)-Incarvillateine Mechanism of Action
6	Sneha Basak	Sneha Basak, Fereidoon Daryaei, Rajeswari Basu, Jonathan Merino, Yiqian Li, James Iuliano, Peter J. Tonge	Time-Dependent Inhibition of LpxC

NO.	PRESENTERS	AUTHORS	TITLE
7	Rajeswari Basu	Rajeswari Basu, Fereidoon Daryaei, Sneha Basak, Jonathan Merino, Peter Tonge	The Role of Turn-over in Coupling Between Residence Time and Post- Antibiotic Effect
8	Michelle Beauvais	Michelle Beauvais, Peter Chupas, John Parise, Daniel O'Nolan, Karena Chapman	In Situ Characterization of Solid State Intermediates of Aqueous Iron Sulfide Metathesis Reaction
9	Surita Bhatia	Surita Bhatia	NSF Graduate Training Program: Quantitative Analysis of Dynamic Structures (QuADS), a Data-Driven Approach for Materials Research
10	John Bickel	John Bickel, Robert Rizzo	Utilizing Statistical and Cheminformatics Methods to Improve De Novo Design in DOCK6
11	Francis Boadi	Francis O. Boadi, Jingling Zhang, Xiaoxi Yu, Surita Bhatia, Nicole S. Sampson	Alternating Ring-Opening Metathesis Polymerization (AROMP) Provides Easy Access to Functional and Fully Degradable Polymers
12	Elizabeth Boon	Elizabeth Boon	NIH Graduate Training Program: SBU Chemistry-Biology Interface Training Program
13	Amanda Carr	Amanda J. Carr, Weiping Liu, Bingqian Zheng, Kevin G. Yager, Alexander R. Routh, Surita R. Bhatia	Probing Complex Stratification Regimes using Novel Micro-Beam X-ray Scattering
14	Danielle Cervasio	Danielle A. Cervasio, Alyssa N. Preston, Isabella R. Pizzuto, Nipuni Gunawardhana, Kevin C. Tan, Scott T. Laughlin	Targeting the Brain's Astrocytes using Diverse Small Molecules
15	Emily Chen	Emily Chen, Bin Sun, Eric Patterson, Nancy S. Goroff	Building Phenylene Ethynylene Macrocycles as 1,4 Diiodobutadiyne Hosts

NO.	PRESENTERS	AUTHORS	TITLE
16	Lei Chen	Lei Chen, Changwei Wang, Wanrong Guo, Xin Wang, Yunrong Jing, Yi Sun, Iwao Ojima	Design, Synthesis, and Biological Evaluations of Next-Generation taxoids, Bearing m-OCF3 and m-OCF2H groups at the C2 Benzoate Moiety
17	Lexin Chen	Lexin Chen, Hongyang Ma, Nisha Verma, Skylar Wu, Benjamin Hsiao	Ionic Liquid Surfactant Assisted Interfacial Polymerization to Fabricate High Flux Composite Reverse Osmosis Membranes
18	Zhihengyu Chen	Zhihengyu Chen, Michelle L. Beauvais, Matthew C. Simons, Louis Redfern, Ying Yang, Jian Liu, Aditya Bhan, Joseph T. Hupp, Omar K. Farha, Karena W. Chapman	Watching How Nanocatalysts Cook at High Temperature
19	Kelley Chiu	Kelley Chiu, Elliot J. Crooks, Martine Ziliox, Toru Kawakami, Tiffany Victor, Feng Xu, Hironobu Hojo, Carlos Simmerling, William E. Van Nostrand, Steven O. Smith, Lisa M. Miller	Copper Stabilization in Anti-Parallel A β 40-Iowa Amyloid Beta Fibrils
20	Matthew Cifone	Matthew Cifone, Yiqian Li, Rajeswari Basu, Craig Stivala, Peter Tonge	Bivalent Inhibitors of Acetyl-CoA Carboxylase
21	Timothy Clement	Timothy Clement, Monaf Awwa, Hehe Wang, Chuanzhou Zhu, Adam Taouil, Antonella Pepe, Huilin Li, Matthew W. Elmes, Martin Kaczocha, Dale G. Deutsch, Iwao Ojima	Design, Synthesis, and SAR Study of Truxillic Acid-Based Fatty Acid Binding Protein Inhibitors as Anti-Nociceptive and Anti-Inflammatory Agents

NO.	PRESENTERS	AUTHORS	TITLE
22	Adam Corrao	Adam Corrao, Christopher Coaty, Gerard Mattei, Victoria Petrova, Zhuo Li, Ping Liu, Peter G. Khalifah	Coarsening in Conversion Reaction Synthesized Nanoporous Metals and Nanocomposites: Insights from In Situ Synchrotron Diffraction Studies
23	Alexia Cosby	Alexia G. Cosby, Gregory Quevado, Eszter Boros	In Situ Excitation of Lanthanide Luminescence for Optical Imaging
24	Monty Cosby	Monty R. Cosby, Yusu Wang, Gerard S. Mattei, Zhuo Li, Karena W. Chapman, Peter J. Chupas, Peter G. Khalifah	In Situ Studies of ion Exchange Reactions of $\text{Na}_2\text{Mg}_2\text{P}_3\text{O}_9\text{N}$: Kinetic and Thermodynamic insights
25	Abbigayle Cuomo	Abbigayle Cuomo, Lauren E. Raguette, Carlos Simmerling	Testing Parameters for Simulation of Phosphorylated Amino Acids
26	Shabnam Davoodi	Shabnam Davoodi, Yiqian Li, James Iuliano, Matthew Cifone, Fereidoon Daryaei, Peter J. Tonge	Target Vulnerability Assessment of Targeted Protein Degradation and Small-Molecule Inhibition
27	Jonathan Denney and Yusu Wang	Jonathan Denney, Yusu Wang, Adam Corrao, Pete Chupas, Peter Khalifah, Hui Zhong, John Trunk, Dan Olds, Eric Dooryhee, Guanglong Huang, David Montiel, Katsuyo Thornton	In Situ Synchrotron Studies of Optical Floating Zone Single Crystal Growth Environments
28	Zachary Fallon	Zachary Fallon, Carlos Simmerling, Miguel Garcia-Diaz	How Does DNA Polymerase Recognize and Fix its Mistakes During DNA Replication?

NO.	PRESENTERS	AUTHORS	TITLE
29	Jiayuan Fu	Jiayuan Fu, Lisa-Marie Nisbett, Bianca Benayoun, Elizabeth Boon	Characterization of a Novel Nitric Oxide Sensing Protein and its Role in Regulating Biofilm Formation in <i>Burkholderia Thailandensis</i>
30	Qinyi Fu	Qinyi Fu, Nisha Verma, Hongyang Ma, Benjamin M. Ocko, Benjamin S. Hsiao	Structural study of Commercial Reverse Osmosis Membranes
31	Han Gao	Han Gao, David M. Connors, Nancy S. Goroff	A New Route Toward Substituted Phenanthro[9,10-c]thiophenes and Related Polymers
32	Aaron Ghebrehiwet	Aaron Ghebrehiwet, Chenwei Liu, David Hewitt, Robert B. Grubbs	Polyglyoxylates and Polypyruvates: Green Polymers with Degradable Backbones
33	Jose Guerra	Jose Guerra, Zachary Fallon, Carlos Simmerling	Investigating the Incorporation of Base Pair Mismatches in DNA Polymerase using Molecular Dynamics
34	Nipuni Gunawardhana	Nipuni Gunawardhana, Danielle Cervasio, Kevin Tan, Isabella Pizzuto, Alyssa Preston, Scott Laughlin	Selectively Activating Gene Transcription in Astrocytes using Methyl-Pyridinium Tagged Doxycycline
35	Steven Hall	Steven Hall, Elizabeth Boon, Miguel Garcia-Diaz	Crystallographic and Spectroscopic Approaches for Studying the Structure of a Novel Nitric Oxide Sensing Protein, NosP
36	Rebecca Hamlyn	Rebecca Hamlyn, Mausumi Mahapatra, Ivan Orozco, Jose Rodriguez, Sanjaya Senanayake, Michael White	Structural and Chemical State of Cesium on Metallic and Oxidized Copper for small molecule conversion
37	Sang uk Han	Sang uk Han, Manoj Kumar, Jonathan G. Rudick	Ring-opening Polymerization of an Isocyanide-containing Cyclic Carbonate Monomer

NO.	PRESENTERS	AUTHORS	TITLE
38	HongRui He	HongRui He, Tomas Rosén, Chengbo Zhan, Ruifu Wang, Shirish Chodankar, Lin Yang, Benjamin Hsiao	Time Resolved Characterization of Metal Ion-Induced Nanocellulose Gelation by Small Angle X-ray Scattering
39	YongLe He	YongLe He, Iva Chitrakar, James Iuliano, Jarrod French, Peter Tonge	Structure Dynamic Study of a BLUF Protein BlsA
40	Ilana Heckler	Ilana Heckler, Elizabeth M. Boon	The Role of a Novel Nitric Oxide Sensing Hemoprotein in the Biofilm Formation and Antibiotic Resistance of <i>Pseudomonas aeruginosa</i>
41	Lisa Housel	Lisa M. Housel, Jianping Huang, Lei Wang, Andrea M. Bruck, Calvin D. Quilty, Alyson Abraham, Diana M. Lutz, Christopher R. Tang, Andrew Kiss, Juergen Thieme, Kenneth J. Takeuchi, Esther S. Takeuchi, Amy C. Marschilok	High-Capacity Vanadium Oxide Electrodes: Effective Recycling through Thermal Treatment
42	Wei Huang	Wei Huang, Pratik Kumar, Scott T. Laughlin	Exploring Chemical Diversity Towards Cyclopropene Scaffolds for Controllable Ligations
43	Xiangyu Huang	Xiangyu Huang, Guilherme Dognani, Pejman Hadi, Benjamin S. Hsiao	Sustainable Biodegradable Cationic Dialdehyde Nanocellulose for Efficient Hexavalent Chromium Removal
44	Grenalynn Ilacas	Grenalynn C. Ilacas, Benjamin S. Hsiao, Robert B. Grubbs	Isolation and Purification of Lignin from Untreated Biomass
45	Haram Im	Haram Im, I. F. Dempsey Hyatt	In Situ Reaction of Aryl Iodine Compounds with Selectfluor reagents and Reactive Intermediate Difluoro Hypervalent Iodine Compounds on Hypervalent Iodine Guided Electrophilic Substitution (HIGES)

NO.	PRESENTERS	AUTHORS	TITLE
46	James Iuliano	James N. Iuliano, Christopher R. Hall, Jinnette Tolentino Collado, SeungYoun Shin, Agnieszka A. Gil, Pavithran Ravindran, Andras Lukacs, James Arimini, Uthama Edupuganthi, Helena A. Woroniecka, Gregory M. Greetham, Michael Towrie, Jared E. Toettcher, Kevin H. Gardner, Jarrod B. French, Carlos L. Simmerling, Stephen R. Meech, Peter J. Tonge	Structural Dynamics of Allosteric Pathways in LOV Photoreceptors
47	Jaehoon Jang	Jaehoon Jang, Dipankar Sahoo, Noel A. Amaro, Francisco I. Caban, Salvatore J. Bracco, Jessica L. Humann, Jonathan G. Rudick	Synthesis of Hydrogen Bonded Polycatenar Mesogens Based on an Oligo(benzyl ether) Motif
48	Samruddhi Jewlikar	Samruddhi Sanjay Jewlikar, Jinnette Tolentino Collado, James Iuliano, Andras Lukacs, Katrin Adamczyk, Sangyeoun Shin, Carlos Simmerling, Stephen R. Meech, Peter J. Tonge	Mutagenesis of LOV domain to understand Photoactivation
49	Ting Jiang	Ting Jiang, Adrian Thompson, Pratik Kumar, Wei Huang, Wei-Siang Kao, Scott T. Laughlin	Modular Enzyme- and Light-Activatable Cyclopropene-Tetrazine Ligation for Spatiotemporal Imaging of Biological Systems

NO.	PRESENTERS	AUTHORS	TITLE
50	Ken Johnson	Ken I. Johnson, Priyanka R. Sharma, Sunil K. Sharma, Benjamin S. Hsiao	Remediation of Ammonium by Nitro-Oxidized Cellulose Nanofibers
51	Ritika Joshi	Ritika Joshi, Sophie Zhang, Tom Lindstrom, Benjamin S. Hsiao	Developing Hydrophobic Cellulosic Membrane for Membrane Distillation
52	Gabrielle Kamm	Gabrielle E. Kamm, Antonin Grenier, Daniel O'Nolan, Michelle Beauvais, Peter J. Chupas, Karena W. Chapman	Cooking the Right Stuff: Synthesis and In Situ Synchrotron-based X-ray Diffraction Characterization of Materials for Energy Storage Applications
53	Jindong Kang	Jindong Kang, Mausumi Mahapatra, Ning Rui, Ivan Orozco, Rui Shi, Sanjaya D. Senanayake, José A. Rodriguez	Growth and Structural Studies of In/Au(111) Alloys and InOx/Au(111) Inverse Oxide/Metal Model Catalysts
54	Wei-Siang (Mark) Kao	Wei-Siang (Mark) Kao, Andrea Meyer, Jiang Ting, Wei Huang, Scott T. Laughlin	Searching for Optimal Bioorthogonal Substrate Pairs for Bioimaging
55	Koushik Kasavajhala	Koushik Kasavajhala, Kenneth Lam, Carlos Simmerling	Improving Replica Exchange MD Efficiency using Structure Reservoirs
56	Debra Keiser and Eugene Chung	Debra A. Keiser, Eugene Chung, Eric V. Patterson	Modeling the Chlorination of Conjugated Steroids
57	Madani Khan	Madani Khan, Junseo Kim, Jenny Gao, Sunil Sharma, Dale Drueckhammer, Benjamin S. Hsiao	Removal of Water Toxins via Ligand-Functionalized Cellulose-Based Membranes

NO.	PRESENTERS	AUTHORS	TITLE
58	Jinwoo Kim	Jinwoo Kim, Diane M. Bogdan, Matthew W. Elmes, Monaf Awwa, Su Yan, Joyce Che, Garam Lee, Dale G. Deutsch, Robert Rizzo, Martin Kaczocha, Iwao Ojima	Synthesis and Neurobiological Evaluations of (-)-Incarvilleine and its Mono Ester
59	Myounwoo Kim	Myounwoo Kim, Racquel C. DeCicco, Nancy S. Goroff	The Synthetic Efforts Toward Topochemical Polymerization to Poly(dicyanodiacetylene)
60	Saerom Kim	Saerom Kim, Krupanandan Haranahalli, Anna Panapakides, Adam Taouil, Monaf Awwa, Iwao Ojima	Discovery of New 2,5,6-trisubstituted benzimidazoles as anti-TB Agents Targeting FtsZ by Quantitative Structure-Activity Relationships (QSAR) Studies
61	John Klecker	John Klecker, Jennifer Guo, Fereidoon Daryaei, Peter Tonge	PK/PD Modeling of Btk Inhibitors in Hematological Malignancies
62	Greta Klejborowska	Greta Klejborowska, Adam Huczyński, Iwao Ojima	Tumor-Targeting Drug Conjugates of Monensin A, Colchicine or their Derivatives
63	Stephen Koch	Stephen A Koch, Daniel Amarante, Jianfeng Jiang, Gina Chiarella, Doris Melgarejo	Fe(CO)(CN) Chemistry: On Earth and in the Heavens
64	Kenneth Lam	Kenneth Lam, Koushik Kasavajhala, Carlos Simmerling	How reliable are RNA Simulations? The Challenges and Advances that Define the Field
65	Joseph Lauher	Joseph Lauher	What's New in Osher?
66	Scott Laverty	Scott Laverty, Stephen Telehany, John Bickel, Robert C. Rizzo	Evaluating Pose Reproduction Success Across Docking Platforms

NO.	PRESENTERS	AUTHORS	TITLE
67	Johnny Lee	Johnny W. Lee, Weijia Zheng, Ming-Yu Ngai	Catalytic Radical Di- and Trifluoromethoxylation of Arenes and Heteroarenes
68	Catherine Leung	Catherine Leung, Krupanandan Haranahalli, Cristina Lazzarini, Yi Sun, Maurizio Del Poeta, Iwao Ojima	SAR of Acylhydrazones as Novel Antifungal Agents
69	Ming-Hao Li	Ming-Hao Li, Xiaoxue Zhang, Erwin London, Daniel P. Raleigh	The Effect of Ca ²⁺ on Membrane-mediated IAPP Amyloid Formation and IAPP Induced Membrane Damage
70	Yong Li	Yong Li, Fereidoon Daryaee, Kaixuan Li, James Iuliano, Peter Tonge	[¹⁸ F]F-CC-292, A Positron Emission Tomography Probe for imaging Bruton's Tyrosine Kinase in vivo
71	Yusong Liu	Yusong Liu, Spencer L. Horton, Jie Yang, J. Pedro F. Nunes, Xiaozhe Shen, Thomas J. A. Wolf, Ruaridh Forbes, Chuan Cheng, Samuel McClung, Bryan Moore, Martin Centurion, Kareem Hegazy, Renkai Li, Ming-Fu Lin, Albert Stolow, Paul Hockett, Tamas Rozgonyi, Philipp Marquetand, Xijie Wang, Thomas Weinacht	Combining Structural and Spectroscopic Probes of Molecular Dynamics
72	Yilin Ma	Yilin Ma, Kenneth Goodman, Jason Wang, Michael White	CO ₂ hydrogenation on Copper Supported Zirconium Oxide Clusters
73	Lakshan Manathunga	Lakshan Manathunga, Alexander Zhyvoloup, Osman Bilsel, Daniel Raleigh	Investigation of Pre-Amyloid Conformational Preferences of Monomeric Human IAPP

NO.	PRESENTERS	AUTHORS	TITLE
74	Kirsten Martin	Kirsten Martin, Alexia Cosby, Piyusha Lotlikar, Eszter Boros	Luminescent Lanthanide Complexes for Targeted Bioimaging Applications with In Situ CRET Excitation
75	Luz Mendez	Luz C. Mendez, Nicole S. Sampson	Identifying Inducers of the Acrosome Reaction in Human Sperm with Synthetic Glycopolymers
76	Jonathan Merino	Jonathan Merino, Fereidoon Daryaei, Chendi Gu, Rajeswari Basu, Sneha Basak, Yiqian Li, Peter J. Tonge	Probing the Molecular Determinants of LpxC Inhibitor Residence Time
77	Matthew Miller and Rehana Akter	Rehana Akter, Matthew E. Miller, Alexander Zhyvoloup, Rebekah L. Bower, Andisheh Abedini, Debbie L. Hay, Daniel P. Raleigh	Rational Design of Non-Amyloidogenic, Bioactive Human Islet Amyloid Polypeptide (IAPP) Analogs with Improved Solubility: A Promising Adjunct to Insulin Therapy
78	Hanna Morales Hernandez	Hanna Morales Hernandez, Anthony Cirri, Christina Kmiotek, Christopher Johnson	Measuring the Electronic Absorption Spectra of Gold Nanoclusters Via Mass Selective UV-Vis Spectroscopy
79	Daeun Noh	Daeun Noh, Alexander Zhyvoloup, Rebekah L Bower, Debbie L. Hay, Daniel P. Raleigh	Analysis of Amylin Consensus Sequences Suggests that Amylin is not Optimized to Minimize Amyloid Formation and Provides Clues to Factors that Modulate Amyloidogenicity
80	Marc Nolan	Marc Nolan, Priyanka R. Sharma, Benjamin Hsiao	Increased Adsorption Capacity of Pb ²⁺ Ions via Sequential Oxidation of Carboxycellulose Nanofibers
81	Jennifer Noorollah and Nirvanie Singh	Jennifer Noorollah, Nirvanie Singh, I. F. Dempsey Hyatt	<i>In-situ</i> Reaction of (Difluoroiodo)arenes for the Hypervalent Iodine-Guided Electrophilic Substitution (HIGES) Reaction

NO.	PRESENTERS	AUTHORS	TITLE
82	Ivan Orozco	Ivan Orozco, Erwei Huang, Ramon A Gutierrez, Zongyuan Liu, Feng Zhang, Mausumi Mahapatra, Jindong Kang, Heath Kersell, Slavomir Nemsak, Pedro J. Ramirez, Sanjaya D. Senanayake, Ping Liu, Jose A. Rodriguez	Hydroxylation of ZnO/Cu(111) Inverse Catalysts Under Ambient Water Vapor and the Water-Gas Shift Reaction
83	Navanjalee Panagoda	Navanjalee Panagoda, Yu-Ching Chen, Tianao Yuan, Joshua Werman, Xinxing Yang, Miguel Garcia-Diaz, Nicole Sampson	Elucidating the Role of the Transcriptional Regulator Mce3R and mel2 Encoded Genes in <i>Mycobacterium tuberculosis</i> Drug Resistance
84	Apurva Pandey	Apurva Pandey, Chloé Savino, Zhaoyong Yang, Stephen VanLanen, Eszter Boros	Gallium based Ciprofloxacin Siderophore-Conjugates with Broad Spectrum Antibiotic Activity
85	Lauren Parrinello	Lauren Parrinello, Paul Venturi, Tomasz Lecki, Dr. Justyna Widera-Kalinowaska, Prof. dr. hab. Magdalena Skompska	Electrochemical Synthesis of WO ₃ Modified with Exfoliated g-C ₃ N ₄ for Visible Light Photocatalytic Degradation of Methyl Orange Dye
86	Jorge Pincay	Jorge Pincay, Yuzhang Wang, Chuan Tian, Koushik Kasavajhala, Carlos Simmerling	Improvement of the Implicit Solvent Model Gbneck2 for MD Simulation
87	Isabella Pizzuto	Isabella R. Pizzuto, Danielle A. Cervasio, Alyssa N. Preston, Kevin C. Tan, Nipuni Guanwardhana, Scott T. Laughlin	Synthesis of Astrocyte-Targeted Doxycycline Probes

NO.	PRESENTERS	AUTHORS	TITLE
88	Lauren Prentis	Lauren E. Prentis, Trent E. Balius, Carol A. Carter, Robert C. Rizzo	Development and Application of Covalent Docking in DOCK6
89	Lauren Raguette	Lauren E. Raguette, Kellon A.A. Belfon, Abbigayle E. Cuomo, Chuan Tian, Qin Wu, Carlos Simmerling.	Amber Parameters for Phosphorylated Amino Acids
90	Joseph Riccardi	Joseph Riccardi, Dale G. Drueckhammer	Synthesis of a Fluorescent Sensor for Calcium Measurement in Marine Sediments
91	Zachary Ridgway	Zachary Ridgway, Daeun Noh, Amy Wong, Rebekah L. Bower, Ann Marie Schmidt, Daniel P. Raleigh	Disulfide and Proline Mutations of IAPP Yield new Insight Into Mechanisms of Misfolding
92	Rui Shi	Rui Shi, Mausumi Mahapatra, Jindong Kang, Ivan Orozco, Sanjaya Senanayake, Jose Rodriguez	Preparation and Characterization of ZrO ₂ /CuOx/Cu(111) Inverse Model Catalyst
93	Fatima Siddiqi	Fatima Siddiqi, I. F. Dempsey Hyatt	Forming Spirolactams to Cure Trichomoniasis Vaginalis
94	Alvaro Sponza Mata	Alvaro Sponza Mata, Di Liu, Dandan Yang, Melanie Chiu	Modulating Polymer Dispersity with Light: Cationic Polymerization of Vinyl Ethers Using Photochromic Initiators
95	Chavis Stackhouse	Chavis A. Stackhouse, Alyson Abraham, Mikaela Dunkin, Bingjie Zhang, Jianping Huang, Paul F. Smith, Esther S. Takeuchi, Amy C. Marschilok, Kenneth J. Takeuchi	Progress and Outlook on Few Component Composite Solid State Electrolytes

NO.	PRESENTERS	AUTHORS	TITLE
96	Killian Tallman	Killian R. Tallman, David C. Bock, Bingjie Zhang, Lei Wang, Xiao Tong, Amy C. Marschilok, Kenneth J. Takeuchi, Esther S. Takeuchi	Surface Modified Graphite Electrodes for Limiting Li-Plating and Enabling Fast Charging of Li-ion Batteries
97	Rodger Tan	Rodger Tan, John Bickel, Hashim Al-Hasimi, Robert Rizzo	Establishing RNA Docking Protocols for DOCK6
98	Adam Taouil	Adam K. Taouil, Monaf Awwa, Timothy Clement, Atri G. Maharaj, Jinwoo Kim, Yi Sun, Antonella Pepe, Huilin Li, Robert C. Rizzo, Matthew W. Elmes, Martin Kaczocha, Iwao Ojima	Design, Synthesis, and Biological Evaluation of the Inhibitors of Fatty Acid Binding Protein 5 as Next-Generation Therapeutics for Chronic Pain and Inflammation
99	Stephen Telehany	Stephen Telehany, Monica Humby, Dwight McGee, Amy Jacobs, Robert C. Rizzo	Virtual Screening Campaign to Identify Small Molecule Inhibitors of Glycoprotein E in Zika Virus
100	Jinnette Tolentino Collado	Jinnette Tolentino Collado, Andras Lukacs, James Iuliano, Katrin Adamczyk, Jarrod B. French, Stephen R. Meech, Peter J. Tonge	Unraveling the Photoactivation Mechanism of The Light Activated Adenylate Cyclase using Unnatural Amino Acid (UAA)
101	Kimberly Tsang	Kimberly Tsang, Eisen C. Gross, Yue Xu, Trevor J. Sears	Re-evaluation of Ortho-Para-Dependence of Self-Pressure Broadening in the v1 + v3 Band of Acetylene
102	Brett Vaughn	Brett A. Vaughn, Shin Hye Ahn, Eduardo Alucio, Justin Devaraj, Aeli P. Olson, Jonathan Engle, Eszter Boros	Radiometal-Based Small Molecule Tracers for Prostate Cancer

NO.	PRESENTERS	AUTHORS	TITLE
103	Nisha Verma	Nisha Verma, Benjamin M. Ocko, Benjamin S. Hsiao	Molecular Structural Study-facilitated Selection of Monomers for Fabricating Reverse Osmosis Polyamide Membranes
104	Jason Wang	Jason Wang, Yilin Ma, Kenneth Goodman, Michael White	STM Studies of the Surface Morphology of Metal Oxide Clusters on Metal Surfaces
105	Ruifu Wang	Ruifu Wang, Tomas Rosen, Chengbo Zhan, Benjamin S. Hsiao	The Morphology and Flowing Behaviors of TEMPO-Oxidized Cellulose Nanofibers Dispersed in Non-Aqueous Solutions
106	Yuzhang Wang	Yuzhang Wang, Chuan Tian, Koushik Kasavajhala, Jorge Pincay, Carlos Simmerling	Comparison of Folding Simulations of Mini-proteins using Different Amber Force Field
107	Joshua Werman	Joshua M. Werman, Tianao Yuan, Yu-Ching Chen, Xinxin Yang, Nicole S. Sampson	Exploiting <i>Mycobacterium tuberculosis</i> Cholesterol Metabolism for New Opportunities in Anti-TB Drug Discovery
108	Shengwei Xiong and SeungYoun Shin	Shengwei Xiong, SeungYoun Shin, Adam Taoil, Monaf Awwa, Greta Klejborowska, Jinwoo Kim, Iwao Ojima	Computer-Aided Design of Novel β -Lactam and Thiazole Analogs of Vascular Disrupting Anticancer Agent, Combretastatin A-4
109	Mengying Yang	Mengying Yang, Pejman Hadi, Hongyang Ma, Harold Walker, Benjamin S. Hsiao	Effect of the Charge Density/ Zeta Potential on the Fouling Reduction of Nanocellulose Coated Ultrafiltration Membranes
110	Yi Yang	Yi Yang, Sarah E. Waller, John J. Kreinbuhl, Christopher J. Johnson	Hydration of Atmospherically-Relevant Sulfuric Acid/Ammonia/Amine Clusters

NO.	PRESENTERS	AUTHORS	TITLE
111	Gabriella Yao	Gabriella Yao, Rehana Akter, Lakshan Manathunga, Ming- Hao Li, Alexander Ziyvoloup, Daniel Raleigh	The Effects of a Primordial Chaperone on Islet Amyloid Formation and Toxicity
112	Gyusaang Youn	Gyusaang Youn, Jakob Cervin, Andrew Boucher, Xiaoxi Yu, Ulf Yrlid, Surita R. Bhatia, Nicole S. Sampson	Multivalent Glycomimetic Polymers with Enhanced Cholera Toxin B Binding Affinity for Novel Cholera Treatment
113	Jackie Zheng	Jackie Zheng, Nancy Li, Pejman Hadi- Myavagh, Meng Ying Yang, Xiang Yu Huang, Harold Walker, Benjamin Hsiao	High Flux Nanocellulose-Embedded Mix Matrix Membranes
114	Junjie Zou	Junjie Zou, Carlos Simmerling, Daniel P. Raleigh	Dissecting the Energetics of Intrinsically Disordered Proteins via a Hybrid Experimental and Computational Approach

Keynote Lecture
Student Activities Center Auditorium, 3:15 p.m.

**From Medical Applications to the Environment:
The Important Role of Energy Storage**

Dr. Esther S. Takeuchi

SUNY Distinguished Professor

William and Jane Knapp Chair in Energy and the Environment

Department of Materials Science and Chemical Engineering

Department of Chemistry

Stony Brook University

Advances in electrochemical energy storage are critical and may be a key factor in the adoption of renewable energy derived from wind and solar installations. Additionally, transportation, personal electronics and biomedical applications have ever increasing demands for portable power. Despite remarkable advances in the optimization of electrochemically active materials over the last several decades, there remains an urgent need to enhance utilization efficiencies and to develop materials that can safely deliver both high power and energy density.

We are pursuing the investigation of factors that influence battery life time as well as those that affect ion and electron transport properties of electroactive materials. Examples in the context of battery applications will be provided. Electron transport will be described through the study of bimetallic materials capable of redox initiated in-situ generation of conductive nano-particles with the formation of a conductive network by reduction displacement reactions. Interfacial effects on ion transport will be described including anode-cathode cross-talk.

Notes on the Speaker



Dr. Esther S. Takeuchi is a SUNY Distinguished Professor and the William and Jane Knapp Chair in Energy and the Environment in the Departments of Materials Science and Chemical Engineering and Chemistry at Stony Brook University. She holds a joint appointment at Brookhaven National Laboratory as Chief Scientist in the Energy and Photon Sciences Directorate. Dr. Takeuchi is a member of National Academy of Engineering, was awarded the National Medal of Technology and Innovation, was inducted into the National Inventors Hall of Fame and is a Charter Member of the National Academy of Innovation. She received the E. V. Murphree Award and Astellas Award from the American Chemical Society and the Electrochemical Society Battery Division Technology award.

She is a Fellow of the Electrochemical Society (ECS) the American Institute of Medical and Biological Engineering (AIMBE) and American Association for the Advancement of Science (AAAS). Dr. Takeuchi is inventor > 150 patents and received the 2018 European Inventor Award in the category of non-EPO countries.

Prior to her academic appointment, she was employed at Greatbatch, Inc., where her research focused on lithium battery research for implantable applications. Her work was instrumental in the success of the lithium/silver vanadium oxide (Li/SVO) battery, the power source enabling the widespread adoption of life-saving implantable cardiac defibrillators (ICDs). She began her academic career at the University at Buffalo in the Departments of Electrical Engineering and Chemical Engineering and relocated to Stony Brook University and Brookhaven National Laboratory in 2012. Dr. Takeuchi received a bachelor's degree from the University of Pennsylvania with a double major in chemistry and history and completed a Ph.D. in chemistry at the Ohio State University.