

OBD Workshop Program

October 13 – 14, 2022 Houston, Texas, USA



GENERAL INFORMATION

Date

October 13-14, 2022

Venue

Elizabeth D. Rockwell Pavilion, MD Anderson Library, 2nd floor 4333 University Drive, Houston, TX 77204, USA

Website: https://orgabattdays.ece.uh.edu/

Chairman

Prof. Yan Yao

Department of Electrical & Computer Engineering and TcSUH, University of Houston, Houston, Texas, USA

Organization Committee

Ms. Susan Butler (University of Houston, USA)

Mr. Ligun Guo (ECS UH Student Chapter, USA)

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Prof. Jodie Lutkenhaus (Texas A&M University, USA)

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Dr. Masaru Yao (National Institute of Advanced Industrial Science and Technology, Japan)

Prof. Yan Yao (University of Houston, USA)





WELCOME

Dear Friends and Colleagues,

Welcome to the 5th Organic Battery Days at the University of Houston on October 13–14, 2022. We are pleased to continue the series of Organic Battery Days events that started in Uppsala, Sweden, in 2017, and this is the first time that Organic Battery Days is being held in the United States!



Building on the success of previous meetings, this year's event aims to strengthen communication and cooperation among experts from academic organizations, research institutes, and manufacturing companies, as well as to exchange knowledge and experience on the most recent developments in the field of organic batteries. The meeting will discuss the design and synthesis of organic electroactive materials, the study of these materials in various electrochemical systems (e.g., rechargeable batteries, flow cells), and electrolytes for organic electrodes. This meeting will be held in person.

Our graduate students and young professionals have generously volunteered their time and talents to help plan and implement this Workshop. They have provided invaluable thought and initiative to assure you will have a meaningful visit and stand ready to assist you during your stay.

I look forward to an inspiring meeting that will generate novel ideas in this exciting field of research and development.

Sincerely,

Yan Yao

OBD2022 Chairman

Hugh Roy and Lillie Cranz Cullen Distinguished Professor, Electrical and Computer Engineering; Texas Center of Superconductivity at the University of Houston (TcSUH), University of Houston



WEDNESDAY 10/12	THURSDAY 10/13	FRIDAY 10/14	SATURDAY 10/15
	7:00 – 8:30 a.m. Breakfast + late registration (Hilton Shamrock BC)	7:00 – 8:30 a.m. Breakfast (Hilton Shamrock BC)	
	9:15 – 9:30 a.m. (ERP) Welcome and Opening Remarks		
	9:30 – 10:10 a.m. (ERP) Plenary Lecture	9:10 – 10:15 a.m. (ERP) Session D: Virtual Poster	
	10:10 – 10:15 a.m. (ERP) Greetings from the University of Houston		
	10:15 – 10:55 a.m. (ERP) Plenary Lecture	10:15 – 10:30 a.m. (ERP) Coffee/Tea Break	
	10:55 – 11:10 a.m. (ERP) Coffee/Tea Break	10:30 – 11:10 a.m. (ERP) Plenary Lecture	
	11:10 am – 12:40 p.m. (ERP) Session A: Material Discovery	11:10 a.m. – 12:40 p.m. (ERP) Session E: Redox Flow Battery	
	12:40 – 2:00 p.m. Lunch Buffet (MD Anderson Library)	12:40 – 2:00 p.m. Lunch Buffet (MD Anderson Library)	
	2:00 – 3:45 p.m. (ERP) Session B: Underlying Mechanism	2:00 – 3:45 p.m. (ERP) Session F: Emerging Applications	8:00 a.m. – 1:30 p.m. NASA/Johnson Space Center Tour
	3:45 – 4:00 p.m. (ERP) Coffee/Tea Break	3:45 – 4:00 p.m. (ERP) Coffee/Tea Break	
2:00 – 6:00 p.m. Registration (Hilton Lobby)	04:00 – 5:45 p.m. (ERP)	4:00 – 5:20 p.m. (ERP) Session G: Physical Properties	
	Session C: Multivalent Systems	5:20 – 5:40 p.m. (ERP) Poster Awards & Closing Remarks	
6:30 – 9:00 p.m. Welcome to Houston BBQ (Student Center Ballroom)	6:30 – 9:00 p.m. Conference Dinner (Hilton Shamrock BC)	7:00 – 9:30 p.m. Board & Invited Speakers' Dinner (Brennan's of Houston)	

(ERP): Elizabeth Rockwell Pavilion – M.D. Anderson Library



OBD WORKSHOP PROGRAM

- Wednesday, OCTOBER 12, 2022

2:00 – 6:00 p.m. **Registration**

Hilton Main Lobby Near Hotel Registration Desk

6:15 p.m. Meet in South Lobby at Main Entrance for Escort to BBQ

6:30 – 9:00 p.m. Welcome to Houston BBQ

Student Center Ballroom – 2nd Floor, New South Wing

Thursday, OCTOBER 13, 2022

Hilton University of Houston

7:00 – 8:30 a.m. Breakfast Buffet Open. Late registration outside room. (Hilton Shamrock BC)

8:30 a.m. Meet in the South Lobby 1st floor for escort to Elizabeth D. Rockwell Pavilion, M.D.

Anderson Library using Lynn Eusan Park Exit

Elizabeth D. Rockwell Pavilion – M.D. Anderson Library

9:00 a.m. Doors open – Take seats

9:15 – 9:30 a.m. Welcome and Opening Remarks

Yan Yao, OBD 2022 Chair, University of Houston & TcSUH, Houston, Texas, USA

Greetings from the UH Cullen College of Engineering

Joseph Tedesco, Dean

9:30 – 10:10 a.m. **PL1 Plenary Lecture**

Polymers for High Power Density Organic Batteries

Kenichi Oyaizu, Waseda University, Japan

10:10 – 10:15 a.m. **Greetings from the University of Houston**

Claudia Neuhauser, Interim Vice Chancellor/Vice President for Research

10:15 – 11:55 a.m. **PL2 Plenary Lecture**

Novel Architectures and Experimental Strategies for Organic Electrical Energy

Storage

Héctor D. Abruña, Cornell University, USA

10:55 – 11:10 a.m. **Coffee/Tea Break**



11:10 a.m. – 12:40 p.m. SESSION A: Material Discovery **Chair: Jodie Lutkenhaus**

11:10 – 11:35 a.m. **IT1 Invited Talk**

Discovering New Organic Electrodes

Chen Liao, Argonne National Laboratory, USA

11:35 a.m. –12:00 p.m. IT2 Invited Talk

Designing Organic Small Molecules for High-Performance Electrode Materials Ji Eon Kwon, Korea Institute of Science and Technology, Republic of Korea

12:00 – 12:15 p.m. **CT1 Contributed Talk**

Four Electron Exchange on Benzene Ring

Klemen Pirnat, National Institute of Chemistry, Slovenia

12:15 – 12:40 p.m. **IT3 Invited Talk**

Chemical and Structural Principles for High-Voltage Organic Li-ion Cathodes: the Case

of Conjugated Sulfonamides and their Derivatives

Alexandru Vlad, Université Catholique de Louvain, Belgium

12:40 – 2:00 p.m. **Lunch Buffet**

Elizabeth D. Rockwell Pavilion

2:00 – 3:45 p.m. Chair: Yanliang Liang

SESSION B: Underlying Mechanism

2:00 – 2:25 p.m. **IT4 Invited Talk**

Polymorphism and Electrochemical Behavior of Organic Electrodes Materials

Philippe Poizot, Université de Nantes, France

2:25 – 2:50 p.m. **IT5 Invited Talk**

Towards the Applicability of Density Functional Tight Binding to Charge Transport in

Quinones in Solution and in the Solid State

Puja Goyal, State University of New York at Binghamton, USA

2:50 – 3:15 p.m. **IT6 Invited Talk**

Polymer Particles Containing Redox-Active Organo-Disulfides and Their Potential

Application in Organic Batteries

Shrayesh N. Patel, University of Chicago, USA

3:15 – 3:30 p.m. **CT2 Contributed Talk**

Halogenated Carboxylates as Organic Anodes for Stable and Sustainable Sodium-Ion

Batteries

Jinghao Huang, George Mason University, USA



3:30 – 3:45 p.m. **CT3 Contributed Talk**

Tuning and Improving Active Electrode Materials Thanks to Organic Chemistry Toolbox

Valentin Gouget, Université de Grenoble Alpes, France

3:45 – 4:00 p.m. **Coffee/Tea Break**

4:00 – 5:45 p.m.

Chair: Alae Eddine Lakraychi

SESSION C: Multivalent Systems

4:00 – 4:25 p.m. **IT7 Invited Talk**

Organic Electrode Materials for Divalent Metal-ion Batteries Zhirong Zhao-Karger, Helmholtz Institute Ulm, Germany

4:25 – 4:40 p.m. **CT4 Contributed Talk**

Organic Magnesium Batteries: The Way to Commercialization?

Yanliang Liang, LiBeyond, USA

4:40 – 4:55 p.m. **CT5 Contributed Talk**

Polymers Derived from Aromatic Dianhydrides as Promising Cathodes for

Rechargeable Ca-Metal Batteries

Olivera Lužanin, University of Ljubljana, Slovenia

4:55 – 5:20 p.m. **IT8 Invited Talk**

Mechanics of Organic Mixed Ionic-Electronic Conductors

Kejie Zhao, Purdue University, USA

5:20 – 5:45 p.m. **IT9 Invited Talk**

Organic/Aqueous Hybrid Electrolytes for Reversible Zn and Al Deposition of

Zn Metal and Zn-Al Alloy Anodes

Ho Seok Park, Sungkyunkwan University, Republic of Korea

6:30 – 9:00 p.m. **Conference Dinner**

- Friday, OCTOBER 14, 2022

Hilton University of Houston

7:00 – 8:30 a.m. Breakfast Buffet Open. Late registration outside room. (Hilton Shamrock BC)

8:30 a.m. Meet in the South Lobby 1st floor for escort to Elizabeth D. Rockwell Pavilion, M.D.

Anderson Library, using Lynn Eusan Park Exit

Elizabeth D. Rockwell Pavilion – M.D. Anderson Library

9:00 a.m. Doors open – Take seats



9:10 – 10:15 a.m. SESSION D: Virtual Poster	Chair: Yan Yao
9:10 – 9:15 a.m.	P1 Poster Presentation Bioinspired and Biodegradable Redox-active Polypeptides: From Ring-opening Polymerization of N-Carboxyanhydrides for Sustainable Energy Storage Shih-Guo Li, Texas A&M University, USA
9:15 – 9:20 a.m.	P2 Poster Presentation Engineered Slide-Ring Materials for Energy Storage Applications Jackson Pope, University of Colorado Boulder, USA
9:20 – 9:25 a.m.	P3 Poster Presentation Bio-based High-Voltage Polyhydroxyanthraquinones as Organic Cathode Material for Batteries Tijs Lap, University of the Basque Country, Spain
9:25 – 9:30 a.m.	P4 Poster Presentation Cyclotetrabenzil Macrocycle Based Lithium-ion Chemistry Jianing Meng, University of Houston, USA
9:30 – 9:35 a.m.	P5 Poster Presentation High Spatial Resolution Quantitative Chemo-Mechanical Mapping of Organic Composite Cathode for Sulfide-Based Solid-State Batteries Qing Ai, Rice University, USA
9:35 – 9:40 a.m.	P6 Poster Presentation Studying Superlithiation with Proton Free Terephthalates Zackary Ashworth, Uppsala University, Sweden
9:40 – 9:45 a.m.	P7 Poster Presentation Building a Full Li-ion Prototype Using a Lithiated Organic Active Material For the Positive Electrode Maxime Nicolas, CEA de Grenoble, France
9:45 – 9:50 a.m.	P8 Poster Presentation Lithium-Phenolate (Metal-)Organic Cathodes Rambabu Darsi, Université Catholique de Louvain, Belgium
9:50 – 9:55 a.m.	P9 Poster Presentation Size-Selective Covalent Organic Framework (COF) Composite Membrane to Overcome the Shuttle Effect in Organic Batteries Erin S. Picton, University of Houston, USA
9:55 – 10:00 a.m.	P10 Poster Presentation Redox Active Disulfide Crosslinked Polymeric Particles For Energy Storage Application Hongyi Zhang, University of Chicago, USA



10:00 – 10:05 a.m. **P11 Poster Presentation**

Using Dynamic Crosslinks in Redox Active Colloids to Enable Electrode Cleaning

Sam Kopfinger, University of Chicago, USA

10:05 – 10:10 a.m. **P12 Poster Presentation**

Machine Learning-Accelerated Multiscale Modeling of Radical-Containing

Polymers for All-Organic Batteries

Riccardo Alessandri, University of Chicago, USA

10:10 – 10:15 a.m. **P13 Poster Presentation**

Effect of Stereoregularity on the Electrochemical Properties of Poly(vinylcarbazole)

Khirabdhi T. Mohanty, Texas A&M University, USA

10:15 – 10:30 a.m. **Coffee/Tea Break**

10:30 a.m. – 12:40 p.m. Chair: Wei Wang

SESSION E: Redox Flow Batteries

10:30 – 11:10 a.m. **P3 Plenary Lecture**

Recent Progress in Aqueous Organic Flow Batteries

Michael J. Aziz, Harvard School of Engineering and Applied Sciences, USA

11:10 – 11:35 a.m. **IT10 Invited Talk**

Atomistic Modelling and Data-driven Approaches for Molecular Discovery

Rajeev S. Assary, Argonne National Laboratory, USA

11:35 a.m. –12:00 p.m. **IT11 Invited Talk**

Reversible Ketone Hydrogenation and Dehydrogenation for Aqueous Organic

Redox Flow Batteries

Ruozhu Feng, Pacific Northwest National Laboratory, USA

12:00 – 12:25 p.m. **IT12 Invited Talk**

Predicting the Solubility of Organic Energy Storage Materials Based on Functional

Group Identity and Substitution Pattern Shiyu Zhang, The Ohio State University, USA

12:15 – 12:40 p.m. **CT6 Contributed Talk**

Investigation of Bipolar Isoindoline Nitroxide Materials for Nonaqueous Redox

Flow Batteries

James P. Blinco, Queensland University of Technology, Australia

12:40 – 2:00 p.m. **Lunch Buffet**

Elizabeth D. Rockwell Pavilion



2:00 – 3:45 p.m. SESSION F: Emerging App	Chair: Philippe Poizot lications of Organic Active Molecules
2:00 – 2:25 p.m.	IT13 Invited Talk Industrial Perspectives on Organic Batteries for Energy Storage Ryan M. Stephens, Shell International Exploration and Production, USA
2:25 – 2:50 p.m.	IT14 Invited Talk Redox Gating Achieves New Electrostatic and Ionic Doping Limits Wei Chen, Argonne National Laboratory, USA
2:50 – 3:05 p.m.	CT7 Contributed Talk Towards an Organic Electrode Without Conductive Carbon for Lithium-ion Battery Vincent Pignier, Université de Picardie Jules Verne, France
3:05 – 3:20 p.m.	CT8 Contributed Talk Soluble Organic Catalysts for Non-Aqueous Lithium-Air Batteries Stéven Renault, Université de Nantes, France
3:20 – 3:45 p.m.	IT15 Invited Talk Bioorganic Films for Cleaner Energy Production Charuksha Walgama, University of Houston, USA
3:45 – 4:00 p.m.	Coffee/Tea Break

4:00 – 5:45 p.m.	Chair: Alexandru Vlad
SESSION G: Physical Properties	

4:00 – 4:25 p.m.	IT16 Invited Talk Improved Rate Performance and Energy Density in Conjugated Polymers with Mixed Ionic-Electronic Conduction Rafael Verduzco, Rice University, USA
4:25 – 4:50 p.m.	IT17 Invited Talk An Ultrafast, Durable, and High-Loading Polymer Anode for Aqueous Zinc-Ion Batteries and Supercapacitors Xiaolei Wang, University of Alberta, Canada
4:50 – 5:05 p.m.	CT9 Contributed Talk Structural Lithium-ion Battery Cathodes based on Organic Redox Active Polymers and Kevlar Aramid Nanofibers Suyash Oka, Texas A&M University, USA
5:05 – 5:20 p.m.	CT10 Contributed Talk Engaging Electrochemists: An Introduction to The Electrochemical Society Shannon C. Reed, The Electrochemical Society, USA



5:20 – 5:40 p.m. **Poster Awards and Closing Remarks**

7:00 – 9:30 p.m. **Board & Invited Speakers' Dinner (Brennan's of Houston)**

Meet in Hilton South Lobby by main entrance for transportation

- Saturday, OCTOBER 15, 2022

NASA/Johnson Space Center Private Tour – Space Center Houston

8:00 a.m. Meet at the sidewalk by the Hilton's main entrance, located at Entrance 4

8:05 – 8:10 a.m. Departure to Space Center Houston

9:00 – 10:30 a.m. Private Tram Experience: visit three NASA sites

10:30 – 12:00 a.m. Exhibits, Theatre

12:00 a.m. – 1:30 p.m. Café and/or gift shop

1:30 p.m. Meet at front entrance to depart for UH Hilton



Notes

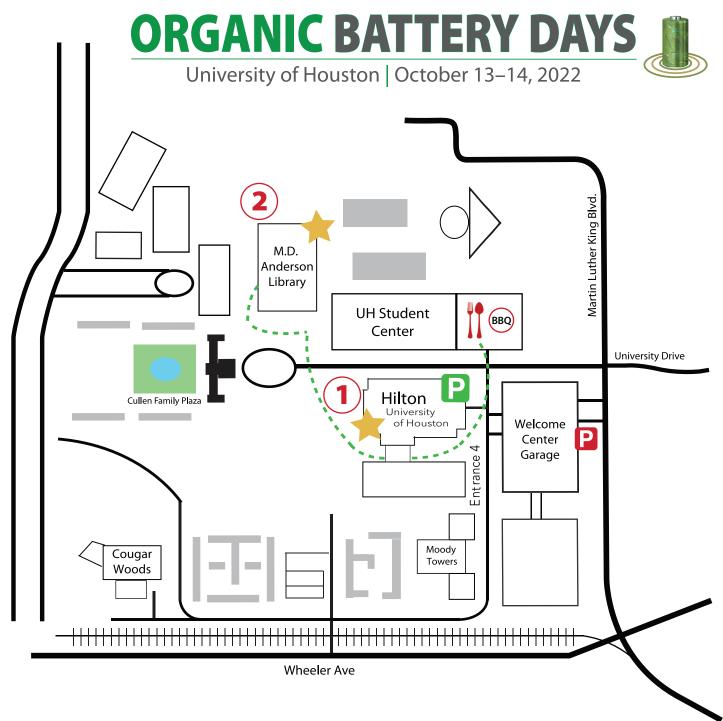


Notes



Notes





OCTOBER 12 - 14, 2022 EVENTS



1 Hotel Registration (10/12) Breakfast Buffet (10/13–14) & Banquet (10/13)

Hilton University of Houston, Shamrock Ballroom 4450 University Drive, Houston, TX 77204



Organic Battery Days – Meeting Location & Lunches (10/13–14)

MD Anderson Library, Elizabeth D. Rockwell Pavilion 2nd Floor – 4333 University Drive, Houston, TX 77204



Welcome BBQ

University Student Center (10/12) 2nd Floor – Ballroom

Parking Garages





Campus Maps: www.uh.edu/maps/

More Parking Information & Rates:

www.uh.edu/parking/parking-on-campus/visitor

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