symposium

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AI-Data Symposium (American Chemical Society, I&EC)

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AI ACS Symposium (https://bit.ly/aiacs)

2025 March 23-27, San Diego, CA & Virtual

This is identical to the original ACS program.

Schedules are in EASTERN TIME!

Sponsored by PMSE, POLY, and I&EC divisions of American Chemical Society

1. Virtual Session -- March 25 Tuesday

Instruction:

Please use your own ACS login to sign in and attend online sessions through ACS meeting site> program tab> my itinerary. Be ready to use Zoom.

The below is from ACS: "Each session opens 10 minutes prior to the start time. Access virtual and live streamed session(s) via My Itinerary in the Full Schedule & My Itinerary tab. Please know that you will need to be registered and be logged into the virtual platform to access these sessions."

Session Chairs: Jie Xu (ANL), Jihua Chen (ORNL), Ngoc Nguyen (UIUC);

1:00 PM - 4:35 PM EST; Tuesday, March 25, 2025

1:00 PM-1:18 PM Autonomous materials informatics for polymer materials development by Yuki Asano

1:18 PM-1:36 PM Practical application of machine learning requires rethinking small data

1:36 PM-1:54 PM withdrawn

1:54 PM-2:12 PM Engineering defect vibrations to enhance interfacial thermal transport in polymer composites

2:12 PM-2:30 PM Direct Sound Printing: 3D printing with ultrasound and holograms and its applications in non-invasive surgery

2:30 PM-2:45 PM withdrawn

2:45 PM-3:03 PM Use of predictive models in advancing biomarkers for precision oncology

3:03 PM-3:21 PM AI for antibiotic discovery

3:21 PM-3:39 PM SMART (synthetic materials and rapid therapeutics): Revolutionizing healthcare and engineering chemistry with AI and data analytics

3:39 PM-3:57 PM Using data science to shed light on zeolite nanoporous structures and how they form

3:57 PM-4:15 PM Withdrawn

4:15 PM-4:33 PM Machine learning to predict designer solvent properties for manufacturing and healthcare applications

Schedules are in EASTERN TIME!

2. In-Person Session -- March 25 Tuesday AM

README

Session Chairs: Wook Shin (Vanderbilt), Miguel Fuentes-Cabrera (NorthEastern Univ.), Qianxiang Ai (MIT)

11:00 AM - 2:15 PM EDT; Tuesday March 25, Room 24B (San Diego Convention Center)

11:00 AM-11:20 AM Atom-pairwise hybrid neural network / physics models for protein-ligand interactions

11:20 AM-11:40 AM AI/ML-driven disease expansion, target selection and candidate selection in drug discovery

11:40 AM-12:00 PM AI and modeling in drug and Vaccine design

12:00 PM-12:20 PM Computational analysis workflows for biological imaging data: data standardization, continual model training, and data storage and sharing

12:20 PM-12:40 PM Machine-learning enhanced photonics engineering for optical transparency in biological tissues

12:40 PM-12:55 PM Break

12:55 PM-1:15 PM Advanced modelling techniques for the optimisation of chromatographic separation processes

1:15 PM-1:35 PM Contrastive learning for drug discovery

1:35 PM-1:55 PM Identifying novel peptide-based therapeutics through AI and simulations

1:55 PM-2:15 PM Role of AI and machine learning in drug discovery and healthcare

3. In-Person Session --- March 25 Tuesday PM

Session Chairs: Zihao Ou (UT Dallas), Sita Sirisha Madugula (ORNL), Wook Shin (Vanderbilt)

5:00 PM - 8:15 PM EDT; Tuesday March 25, Room 24B (San Diego Convention Center)

5:00 PM-5:20 PM Automated analysis of time-dependent specular neutron reflectometry from thin films of ionic polymers using neural networks

5:20 PM-5:40 PM Smart platform for solution processing electronic polymer thin films

5:40 PM-6:00 PM Harnessing DfT and machine learning for accurate optical gap prediction in conjugated polymers

6:00 PM-6:20 PM Advanced manufacturing of wearable sensors for accessible, personalized health monitoring

6:20 PM-6:40 PM Quest to replace Ir as a catalyst for the oxygen evolution reaction

6:40 PM-6:55 PM Break

6:55 PM-7:15 PM Extreme-scale multi-fidelity computational active learning paradigm to realize autonomous synthesis of 2D layered thin-film systems

7:15 PM-7:35 PM Challenges and opportunities in building an autonomous solid state chemistry laboratory (Withdrawn ?)

7:35 PM-7:55 PM Design of AI-guided materials acceleration platforms for emerging semiconductor applications

7:55 PM-8:15 PM Multiscale modeling and data-driven material by design for multifunctional polymers

4. In-Person Session --- March 26 Wednesday AM

Session Chairs: Yifei Jin (Univ. of Nevada-Reno), Hanyu Wang (ORNL), Zihao Ou (UT Dallas)

11:00 AM - 3:00 PM EDT; Wednesday March 26, Room 29C (San Diego Convention Center)

11:00 AM-11:02 AM Opening Remarks By Prof Gobet Advincula

11:02 AM-11:19 AM Digital twin for Chemical Sciences (DTCs): A blueprint for digitizing chemical characterization

11:19 AM-11:36 AM Towards predictive synthesis with atomistic simulations and robust machine learning

11:36 AM-11:53 AM Navigation of digital chemical spaces

11:53 AM-12:10 PM AI/ML optimization workflows of materials properties and manufacturing: importance of autonomous laboratories and data mining

12:10 PM-12:27 PM Functional monomer design via the open macromolecular genome

12:27 PM-12:44 PM Embedded 3D bioprinting: From material design to method development

12:44 PM-1:01 PM Application of Noise2Noise algorithm for high-throughput AFM imaging of polymer membranes

1:01 PM-1:16 PM Break

1:16 PM-1:33 PM Labs of the future: Creating a systems of systems ecosystem for cross-domain scientific autonomous workflows

1:33 PM-1:50 PM Uncertainty characterization of foundation models for reliable applications in materials and Chemistry

1:50 PM-2:07 PM Data-driven design of reactive technologies: Case studies in energy storage

2:07 PM-2:24 PM Opportunities for overcoming the “valley of death” in developing new functional materials

2:24 PM-2:41 PM Modeling nonequilibrium reactive systems with REACTER

2:41 PM-2:58 PM Polymer informatics with large language models

5. In-Person Session --- March 26 Wednesday PM

Session Chair: Sita Sirisha Madugula (ORNL), Qianxiang Ai (MIT), Hanyu Wang (ORNL)

5:00 PM - 8:00 PM EDT; Wednesday March 26, Room 29C (San Diego Convention Center)

5:00 PM-5:05 PM Opening remarks

5:05 PM-5:25 PM Flow visualization and mixing enhancement in Y-junction microchannel with 3D acoustic streaming flow patterns induced by trapezoidal triangular structure using high-viscous liquids

5:25 PM-5:45 PM Designing conjugated polymers with narrow band gap for optoelectronic applications

5:45 PM-6:05 PM Materials informatics for structure-property pelationships (MISPR) for electrolyte and electrode-electrolyte interfaces

6:05 PM-6:25 PM Data-driven approaches to engineer bidomain enzymes

6:25 PM-6:40 PM Break

6:40 PM-7:00 PM ACEG-GNN: Can graph neural network learn to explain activity cliffs?

7:00 PM-7:20 PM Schedule optimization and simulation for chemical library synthesis

7:20 PM-7:40 PM Towards autonomous laboratory workflow for copolymerization: tools, models, ML and LLM

7:40 PM-8:00 PM Machine learning for nanoparticle design

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