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

AI @ American Chemical Society meeting 2025 March 23-27, San Diego, CA & Virtual (Sponsored by I&EC, PMSE, and POLY): The official ACS program is in Eastern Time , but the following program is in Pacific Time:

Session Type	# of talks	Min.	Date	Start Time	End Time	Location
Oral - Virtual	11	215	Tuesday 3/25/2025	10:00 AM	1:35 PM	Digital Session (Digital Meeting)
Oral - In-person	9	195	Tuesday 3/25/2025	2:00 PM	5:15 PM	Room 24B (San Diego Convention Center)
Oral - In-person	9	195	Tuesday 3/25/2025	8:00 AM	11:15 AM	Room 24B (San Diego Convention Center)
Oral - In-person	8	180	Wednesday 3/26/2025	2:00 PM	5:00 PM	Room 29C (San Diego Convention Center)
Oral - In-person	13	240	Wednesday 3/26/2025	8:00 AM	12:00 PM	Room 29C (San Diego Convention Center)

1. March 25 Tuesday, Virtual Session:

Session Chairs: Jie Xu (ANL), Hanyu Wang (ORNL), Ngoc Nguyen (UIUC)

Title	Presenting Author
Autonomous materials informatics for polymer materials development	Shiomi, Junichiro
Practical application of machine learning requires rethinking small data	Yang, Qian
Machine learning guided recognition of halogenated compounds in mass spectrometry-based exposomics	Huan, Tao
Engineering defect vibrations to enhance interfacial thermal transport in polymer composites	Xu, Yanfei
Direct Sound Printing: 3D printing with ultrasound and holograms and its applications in non-invasive surgery	Habibi, Mohsen
Break	
Use of predictive models in advancing biomarkers for precision oncology	Nirmala, Nanguneri
AI for antibiotic discovery	de la Fuente, Cesar
SMART (synthetic materials and rapid therapeutics): Revolutionizing healthcare and engineering chemistry with AI and data ana...	Bhowmik, Debsindhu
Using data science to shed light on zeolite nanoporous structures and how they form	Auerbach, Scott
Molecular insights into room-temperature decomposition of the ethaline deep eutectic solvent using machine learning interatomi...	Yang, Julia
Machine learning to predict designer solvent properties for manufacturing and healthcare applications	Mood, Mohan

Presenting Author	Order	Start Time	End Time	Day/Date
Shiomi, Junichiro	1	10:00 AM	10:18 AM	Tuesday 3/25/2025
Yang, Qian	2	10:18 AM	10:36 AM	Tuesday 3/25/2025
Huan, Tao	3	10:36 AM	10:54 AM	Tuesday 3/25/2025
Xu, Yanfei	4	10:54 AM	11:12 AM	Tuesday 3/25/2025
Habibi, Mohsen	5	11:12 AM	11:30 AM	Tuesday 3/25/2025
	6	11:30 AM	11:45 AM	Tuesday 3/25/2025
Nirmala, Nanguneri	7	11:45 AM	12:03 PM	Tuesday 3/25/2025
de la Fuente, Cesar	8	12:03 PM	12:21 PM	Tuesday 3/25/2025
Bhowmik, Debsindhu	9	12:21 PM	12:39 PM	Tuesday 3/25/2025
Auerbach, Scott	10	12:39 PM	12:57 PM	Tuesday 3/25/2025
Yang, Julia	11	12:57 PM	1:15 PM	Tuesday 3/25/2025
Mood, Mohan	12	1:15 PM	1:33 PM	Tuesday 3/25/2025

Note: The above is the official ACS program. However there are the following changes:

*** The third talk (original scheduled for Prof. Huan Tao) is now by Dr. Jeremy Smith from ORNL on "AI and modeling in drug and Vaccine design".**

*** The break is now canceled. Instead, Prof Aram Amassian (NC State) will talk on "Design of AI-guided materials acceleration platforms for emerging semiconductor applications", starting at 11:30. All talks afterwards will have a 3 minute delay.**

2. March 25 Tuesday, AM In-Person Session

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

Atom-pairwise hybrid neural network / physics models for protein-ligand interactions	Sherrill, Charles
AI/ML-driven disease expansion, target selection and candidate selection in drug discovery	Oprea, Tudor
AI and modeling in drug and vaccine design	Smith, Jeremy
Computational analysis workflows for biological imaging data: data standardization, continual model training, and data storage a...	vasudevan, rama
Machine-learning enhanced photonics engineering for optical transparency in biological tissues	Ou, Zihao
Break	
Advanced modelling techniques for the optimisation of chromatographic separation processes	Michalopoulou, Foteini
Contrastive learning for drug discovery	Glaser, Jens
Identifying novel peptide-based therapeutics through AI and simulations	Perez, Alberto
Role of AI and machine learning in drug discovery and healthcare	Madugula, Sita Sirisha

Sherrill, Charles	1	8:00 AM	8:20 AM	Tuesday 3/25/2025
Oprea, Tudor	2	8:20 AM	8:40 AM	Tuesday 3/25/2025
Smith, Jeremy	3	8:40 AM	9:00 AM	Tuesday 3/25/2025
vasudevan, rama	4	9:00 AM	9:20 AM	Tuesday 3/25/2025
Ou, Zihao	5	9:20 AM	9:40 AM	Tuesday 3/25/2025
	6	9:40 AM	9:55 AM	Tuesday 3/25/2025
Michalopoulou, Foteini	7	9:55 AM	10:15 AM	Tuesday 3/25/2025
Glaser, Jens	8	10:15 AM	10:35 AM	Tuesday 3/25/2025
Perez, Alberto	9	10:35 AM	10:55 AM	Tuesday 3/25/2025
Madugula, Sita Sirisha	10	10:55 AM	11:15 AM	Tuesday 3/25/2025

Note: The above is the official ACS program. However there is the following change:

The third talk (original scheduled for Dr. Jeremy Smith) is now in our virtual session (Mar 25).

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

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

Automated analysis of time-dependent specular neutron reflectometry from thin films of ionic polymers using neural networks	Kumar, Rajeev
Smart platform for solution processing electronic polymer thin films	Xu, Jie
Harnessing DfT and machine learning for accurate optical gap prediction in conjugated polymers	Liu, Mingjie
Advanced manufacturing of wearable sensors for accessible, personalized health monitoring	Ray, Tyler
Quest to replace Ir as a catalyst for the oxygen evolution reaction	Huang, Jin
Break	
Extreme-scale multi-fidelity computational active learning paradigm to realize autonomous synthesis of 2D layered thin-film syst...	Ganesh, Panchapakesan
Challenges and opportunities in building an autonomous solid state chemistry laboratory	Bridges, Craig
Design of AI-guided materials acceleration platforms for emerging semiconductor applications	Amassian, Aram
Multiscale modeling and data-driven material by design for multifunctional polymers	Xia, Wenjie

Kumar, Rajeev	1	2:00 PM	2:20 PM	Tuesday 3/25/2025
Xu, Jie	2	2:20 PM	2:40 PM	Tuesday 3/25/2025
Liu, Mingjie	3	2:40 PM	3:00 PM	Tuesday 3/25/2025
Ray, Tyler	4	3:00 PM	3:20 PM	Tuesday 3/25/2025
Huang, Jin	5	3:20 PM	3:40 PM	Tuesday 3/25/2025
	6	3:40 PM	3:55 PM	Tuesday 3/25/2025
Ganesh, Panchapakesan	7	3:55 PM	4:15 PM	Tuesday 3/25/2025
Bridges, Craig	8	4:15 PM	4:35 PM	Tuesday 3/25/2025
Amassian, Aram	9	4:35 PM	4:55 PM	Tuesday 3/25/2025
Xia, Wenjie	10	4:55 PM	5:15 PM	Tuesday 3/25/2025

Note: The above is the official ACS program. However there is the following change:

The second-to-last talk by Prof Aram Amassian (NC State) on "Design of AI-guided materials acceleration platforms for emerging semiconductor applications" is now moved to our virtual session (March 25).

The third-to last talk was withdrawn.

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

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

Title	Presenting Author
Opening Remarks By Prof Gobet Advincula	
Digital twin for Chemical Sciences (DTCs): A blueprint for digitizing chemical characterization	Qian, Jin
Towards predictive synthesis with atomistic simulations and robust machine learning	Schwalbe Koda, Daniel
Navigation of digital chemical spaces	Colon, Yamil
AI/ML optimization workflows of materials properties and manufacturing: importance of autonomous laboratories and data mining	Advincula, Rigoberto
Functional monomer design via the open macromolecular genome	Jackson, Nicholas
Embedded 3D bioprinting: From material design to method development	Jin, Yifei
Application of Noise2Noise algorithm for high-throughput AFM imaging of polymer membranes	Wang, Qianshu
Break	
Labs of the future: Creating a systems of systems ecosystem for cross-domain scientific autonomous workflows	Moore, Robert
Uncertainty characterization of foundation models for reliable applications in materials and Chemistry	Vital Brazil, Emilio
Data-driven design of reactive technologies: Case studies in energy storage	Spotte-Smith, Evan
Opportunities for overcoming the "valley of death" in developing new functional materials	Kulkarni, Ambar
Modeling nonequilibrium reactive systems with REACTER	Gissinger, Jacob
Polymer informatics with large language models	Agarwal, Sakshi

	1	8:00 AM	8:02 AM	Wednesday 3/26/2025
Qian, Jin	2	8:02 AM	8:19 AM	Wednesday 3/26/2025
Schwalbe Koda, Daniel	3	8:19 AM	8:36 AM	Wednesday 3/26/2025
Colon, Yamil	4	8:36 AM	8:53 AM	Wednesday 3/26/2025
Advincula, Rigoberto	5	8:53 AM	9:10 AM	Wednesday 3/26/2025
Jackson, Nicholas	6	9:10 AM	9:27 AM	Wednesday 3/26/2025
Jin, Yifei	7	9:27 AM	9:44 AM	Wednesday 3/26/2025
Wang, Qianshu	8	9:44 AM	10:01 AM	Wednesday 3/26/2025
	9	10:01 AM	10:16 AM	Wednesday 3/26/2025
Moore, Robert	10	10:16 AM	10:33 AM	Wednesday 3/26/2025
Vital Brazil, Emilio	11	10:33 AM	10:50 AM	Wednesday 3/26/2025
Spotte-Smith, Evan	12	10:50 AM	11:07 AM	Wednesday 3/26/2025
Kulkarni, Ambar	13	11:07 AM	11:24 AM	Wednesday 3/26/2025
Gissinger, Jacob	14	11:24 AM	11:41 AM	Wednesday 3/26/2025
Agarwal, Sakshi	15	11:41 AM	11:58 AM	Wednesday 3/26/2025

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

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

Flow visualization and mixing enhancement in Y-junction microchannel with 3D acoustic streaming flow patterns induced by trap...	Ali, Ayalew
Designing conjugated polymers with narrow band gap for optoelectronic applications	Rai, Neeraj
Materials informatics for structure-property pelationships (MISPR) for electrolyte and electrode-electrolyte interfaces	Rajput, Nav Nidhi
Data-driven approaches to engineer bidomain enzymes	Yang, Zhongyue
Break	
ACEG-GNN: Can graph neural network learn to explain activity cliffs?	Chen, Xu
Schedule optimization and simulation for chemical library synthesis	Ai, Qianxiang
Towards autonomous laboratory workflow for copolymerization: tools, models, ML and LLM	Ivanov, Ilia | Advincula,
Machine learning for nanoparticle design	Reker, Daniel

Ali, Ayalew	2	2:05 PM	2:25 PM	Wednesday 3/26/2025
Rai, Neeraj	3	2:25 PM	2:45 PM	Wednesday 3/26/2025
Rajput, Nav Nidhi	4	2:45 PM	3:05 PM	Wednesday 3/26/2025
Yang, Zhongyue	5	3:05 PM	3:25 PM	Wednesday 3/26/2025
	6	3:25 PM	3:40 PM	Wednesday 3/26/2025
Chen, Xu	7	3:40 PM	4:00 PM	Wednesday 3/26/2025
Ai, Qianxiang	8	4:00 PM	4:20 PM	Wednesday 3/26/2025
Ivanov, Ilia | Advincula, ...	9	4:20 PM	4:40 PM	Wednesday 3/26/2025
Reker, Daniel	10	4:40 PM	5:00 PM	Wednesday 3/26/2025

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