CoC & CoE's ChBE Research Mixer

Research highlights from the faculty of the College of Computing and the College of Engineering's School of Chemical and Biomolecular Engineering

Friday, April 18th, 2025

Georgia Tech

List of Presenters

1. Cindy Xion Bearfield; yxiong82@gatech.edu
2. Alex Duncan; alex.duncan@gatech.edu
3. Yunan Luo; yluo428@gatech.edu
4. Ashutosh Dhekne; dhekne@gatech.edu
5. Martha Grover; mg200@gatech.edu
6. Bjarne Kreitz; bkreitz3@gatech.edu
7. Nian Liu; nliu82@gatech.edu
8. Sankar Nair; sankar.nair@chbe.gatech.edu
9. Patritsia Stathatou; pstathatou3@gatech.edu
10. Julia Yang; jyang317@gatech.edu
11. Jeff Young; jyoung9@gatech.edu
12. Nga Lee (Sally) Ng; ng@chbe.gatech.edu
13. Yibo Hu; yibo.hu@gatech.edu

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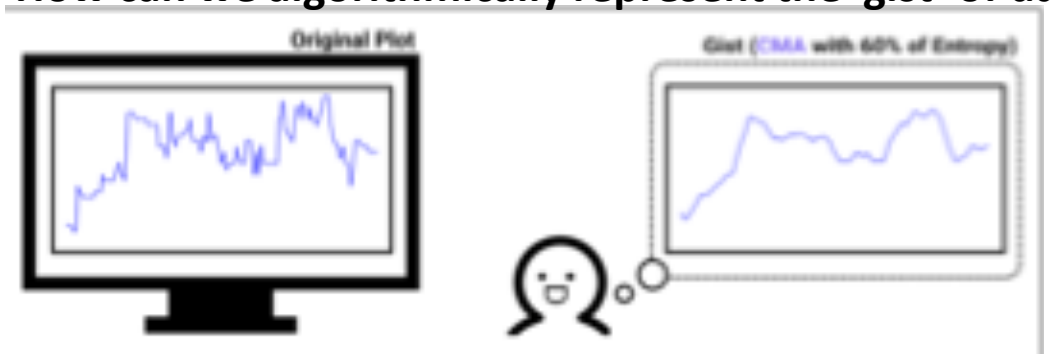
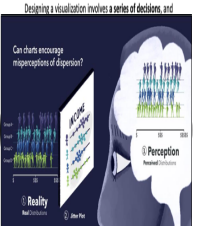
How can we leverage the strength of human perception and cognition to design better visualizations?

How can we algorithmically represent the ‘gist’ of data?

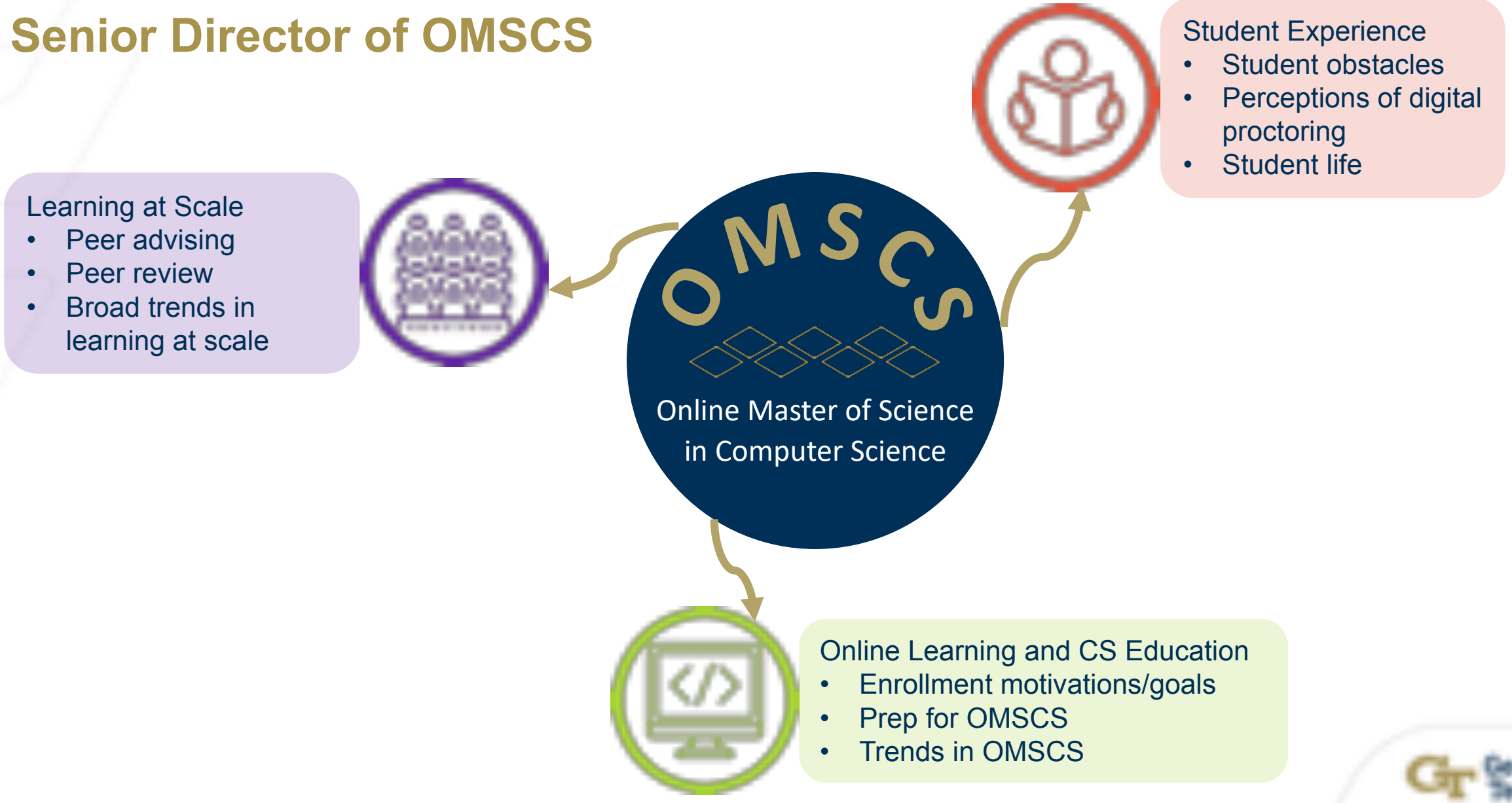


How do we design ‘trustworthy’ visualizations to support reasoning and decision making?

How does visualization design shape public opinion?



Alex Duncan
Senior Director of OMSCS



AI-enabled Protein Engineering/Design

Yunan Luo
Assistant Professor (CSE)
yunan@gatech.edu

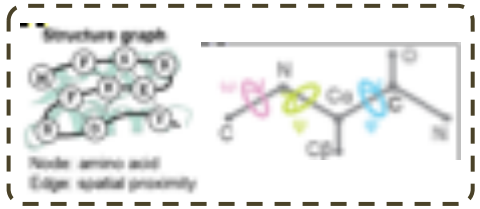
Protein sequence or structure
x

Function prediction
$x \rightarrow f_\theta(\mathrm{x}) \rightarrow y$

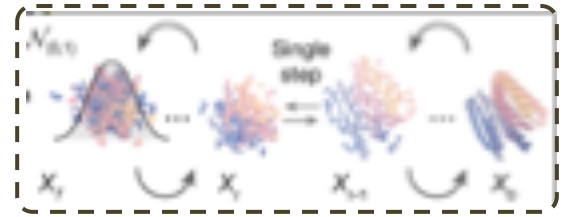
Protein engineering
$x^* \leftarrow \mathrm{argmax}_x f(x)$

Protein function
y

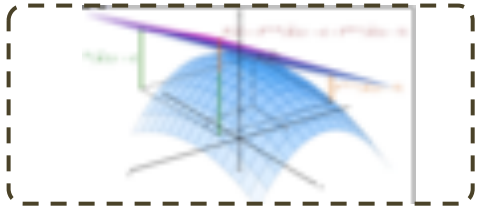
Geometric deep learning



Generative AI



High-dim optimization



Data-efficient language models

Protein function annotation

Enzyme function prediction (*Science*, '23)
Drug-kinase binding prediction (*Nat. Mach. Intell.*, '23)

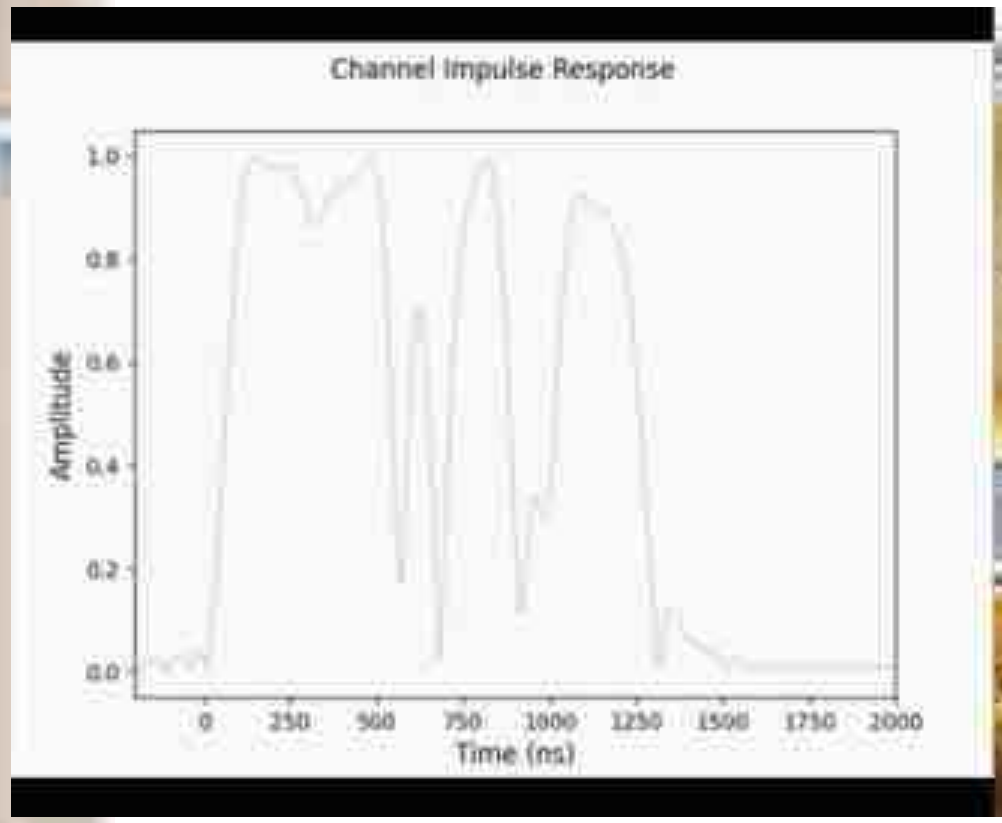
Sequence-fitness prediction

Cold-start enzyme engineering (*Nat Commun, '24)*
Low-*N* protein fitness prediction *(RECOMB, '24)*
Stability change prediction (*RECOMB*, '25)

AI-guided protein engineering/design

Multi-objective protein design (*iScience*, '25)
Small-molecule design (*ICLR*, '25)
Immune complex modelling (*ICML*, '24)

A solid-liquid state transition sensor for water-based substances



Why it works?

The complex permittivity of water and ice is very different at microwave frequencies.

That affects wireless reflections!

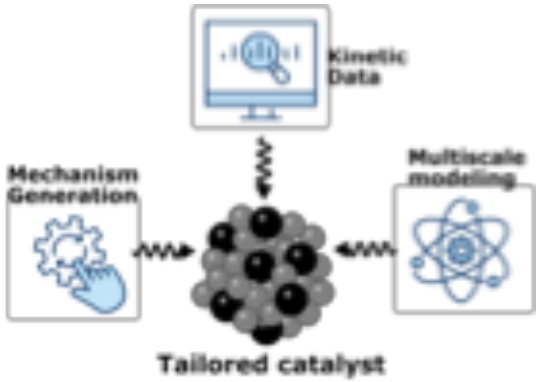
Ashutosh Dhekne
dhekne@gatech.edu

Research in the Kreitz Group

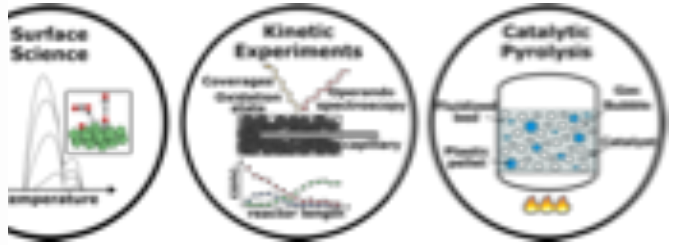
Ab-initio based automated reaction mechanisms development for intricat active site motifs

ng first-principles-based ale modeling of heterogeneously d reactions

Theory Guided Catalyst Design

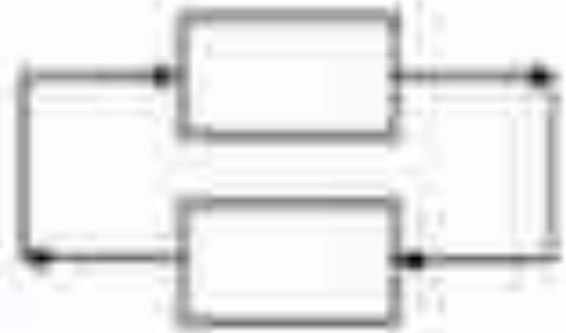


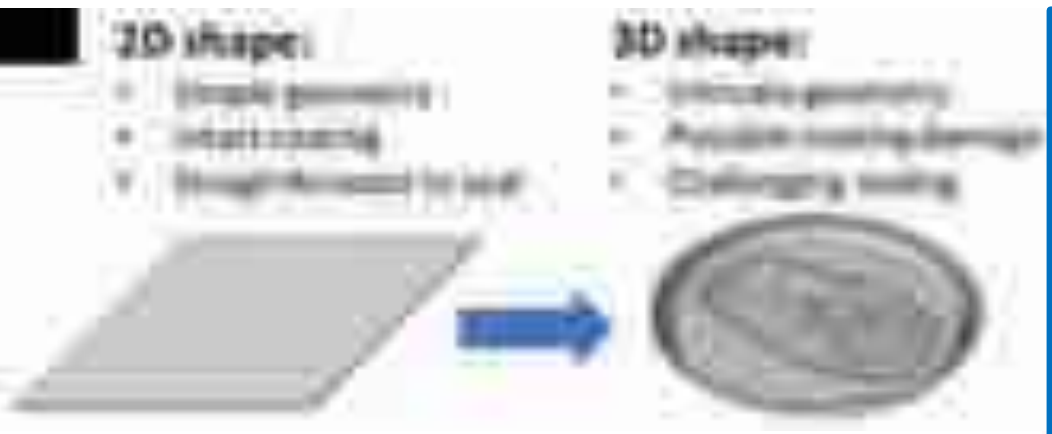
Kinetic Experiments over Well-Defined Catalysts



Grover Group Themes

- Morphology
- Dynamics
- Feedback control

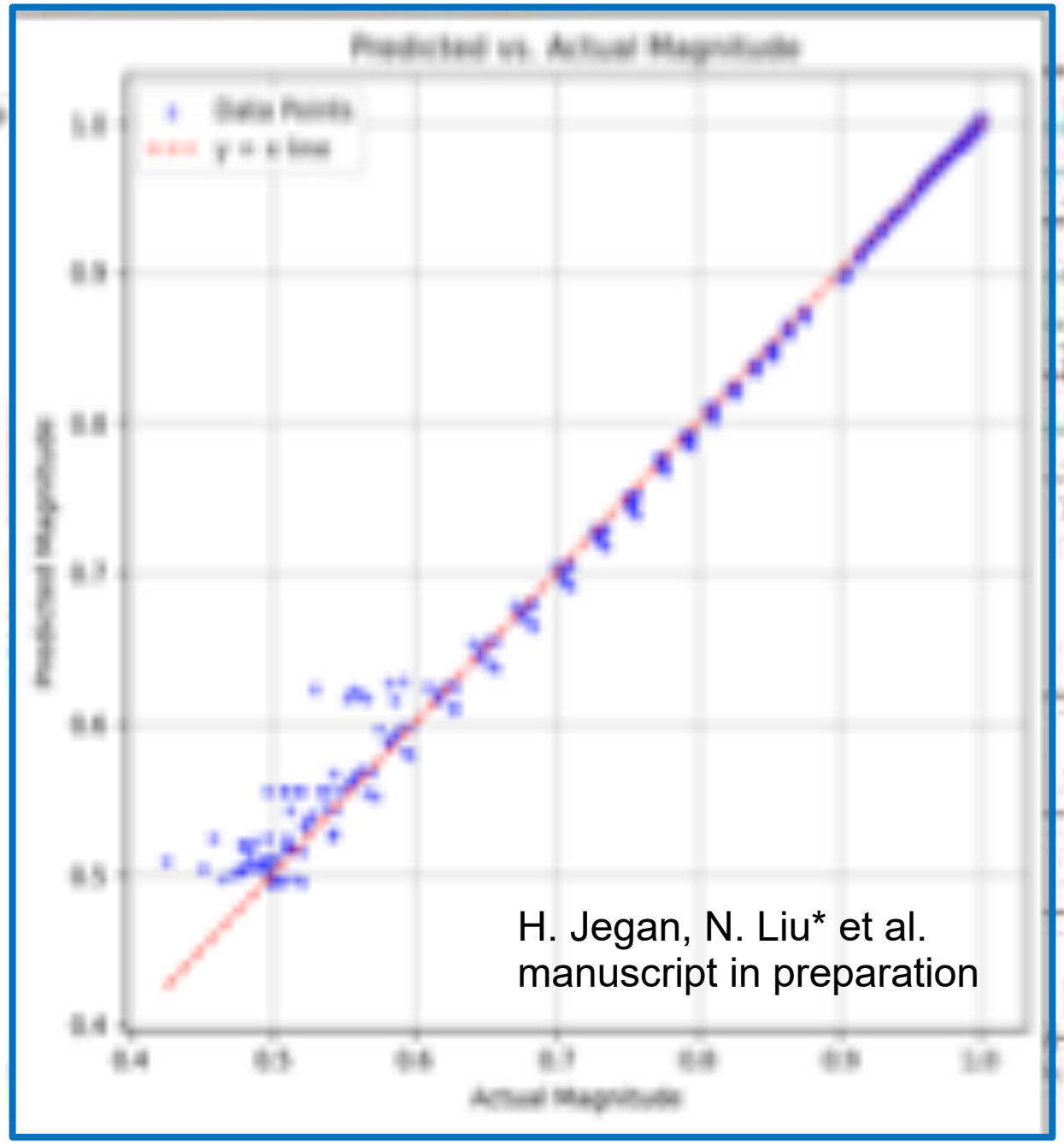




Predict shelf life using e-chem impedance spectroscopy **+ machine learning**

Workflow:

1. Beverage in reactor for electrochemical impedance measurements
2. Identify circuit models using parameters to get data to be simulated
3. Simulate data for model – changing parameters linearly
4. Add Gaussian Noise to mimic experimental data
5. Sequence padding
6. LSTM model predicting temporal data



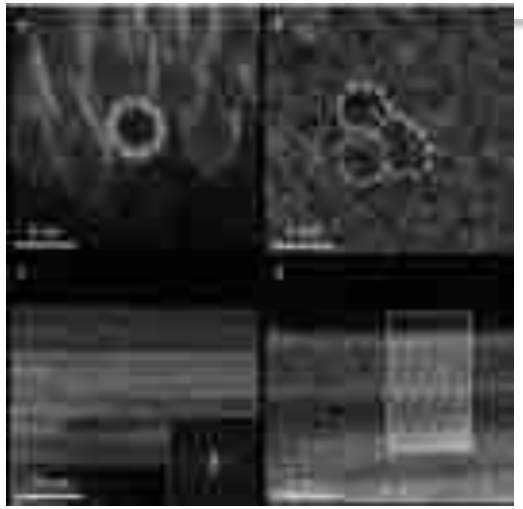
H. Jegan, N. Liu* et al.
manuscript in preparation

Contact Prof. Nian Liu at ChBE:
nian.liu@chbe.gatech.edu

A. Filippas, N. Liu* et al. ***Food Packaging and Shelf Life*** 2024, 44, 101321

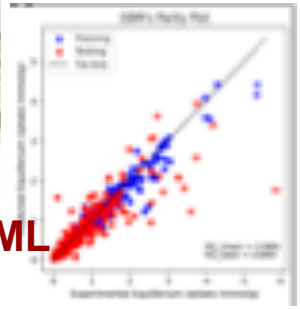
Our Unique Expertise and Infrastructure

We integrate Nanoporous materials and Separation sciences with Applications and Processes

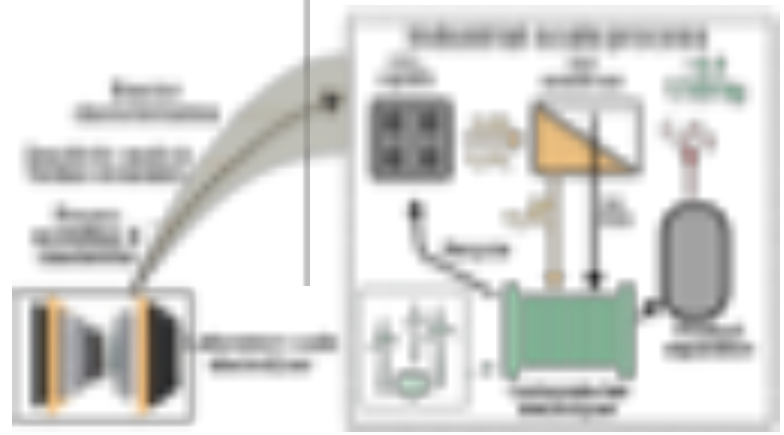


Zeolite nanotubes
Science, 2022

Graphene oxide membranes
Nature Sustainability, 2021



Automated adsorption measurements and ML models in nanoporous carbons



Carbonates-to-chemicals electrolytic processes
Nature Chemical Engineering, 2024

The Stathatou Lab - ASSET

Assessing Sustainable Systems & Emerging Technologies

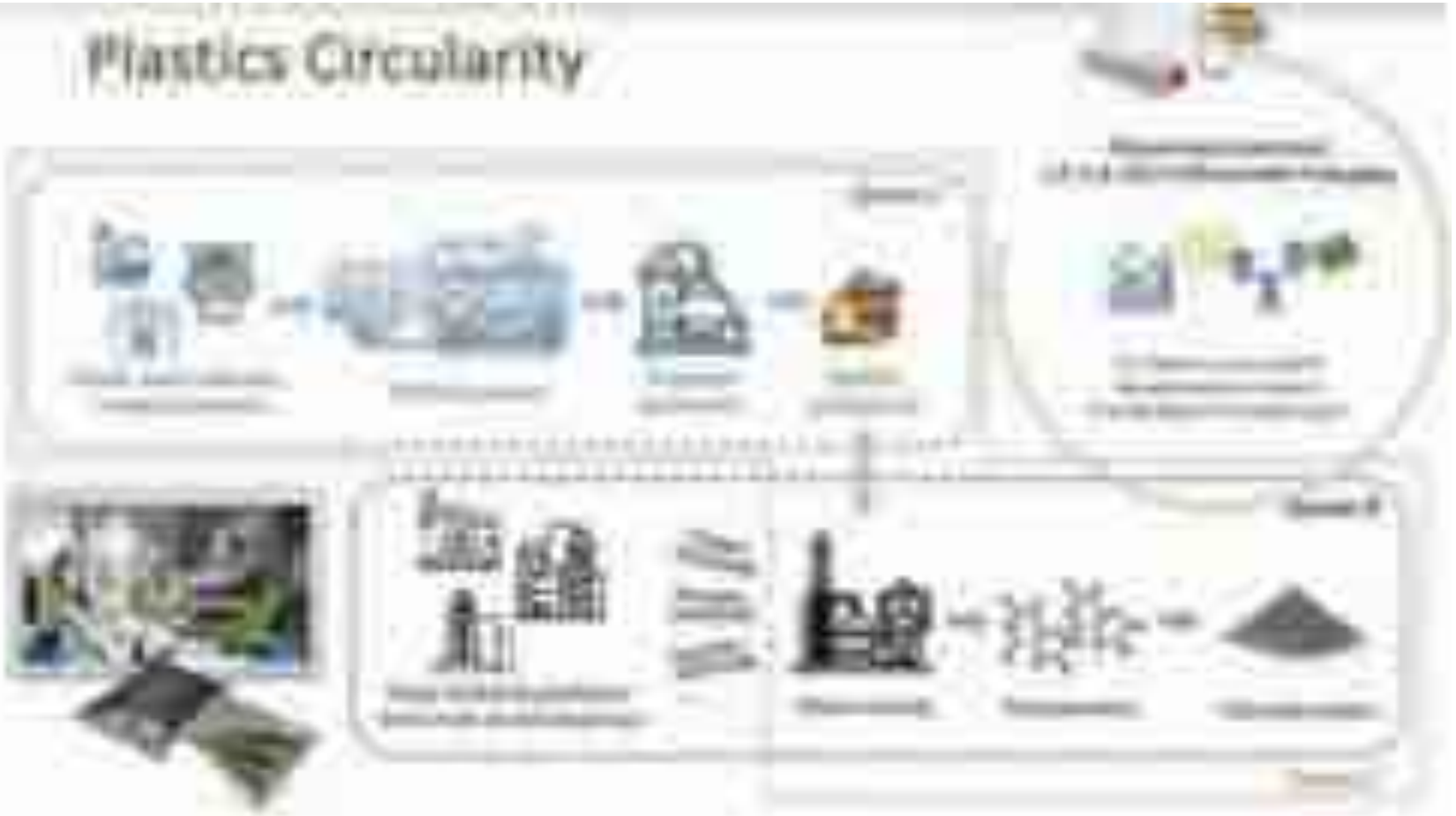
Alternative Fuels & Emission Abatement Technologies

- ✓ Map & model production pathways
- ✓ Design experiments & collect field data
- ✓ Evaluate extensive list of LCA indicators
- ✓ Compare LCA & TEA metrics to BAU scenarios
- ✓ Suggest methodological approaches

Georgia Tech

Plastics Circularity

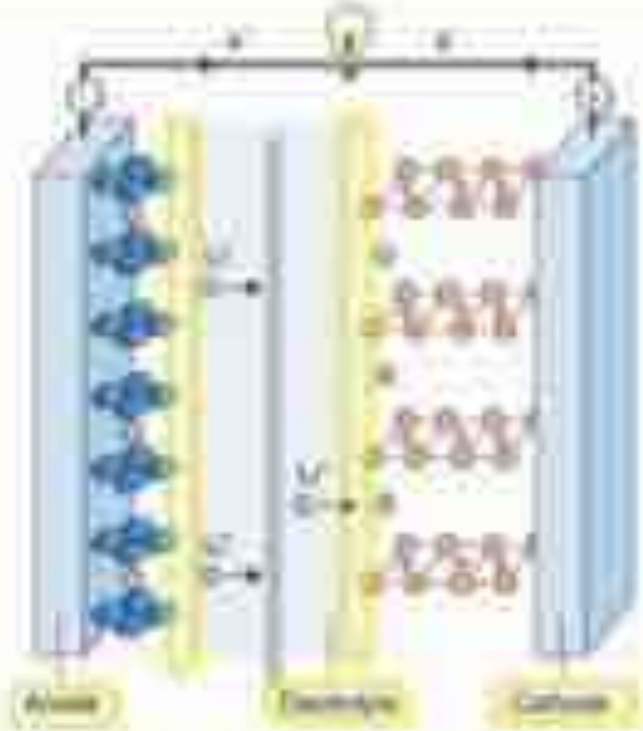
- Assess long-term environmental & economic impacts of multiple recycling cycles & different end-of-life scenarios
- Collect primary data – field measurements
- Evaluate amounts of virgin replenishment
- Identify hotspots in the recycling process
- Compare to virgin plastics production



Emerging Contaminants & Critical Materials

Yang Lab: Sustainable Pathways to Electrification

Team: Xingjiang Ruo, Nicolas Wong, Stella McWhorter, Dr. Julia H. Yang
sites.gatech.edu/[illegible] Lab



1. Chemo-mechanics of polycrystalline electrodes using physics-based ML potentials[1,2,3]

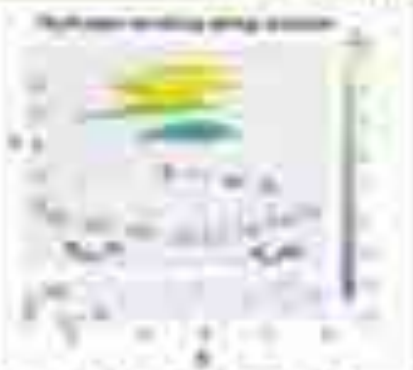
2. Electrolyte discovery for high-performance electrodes[4,5,6]

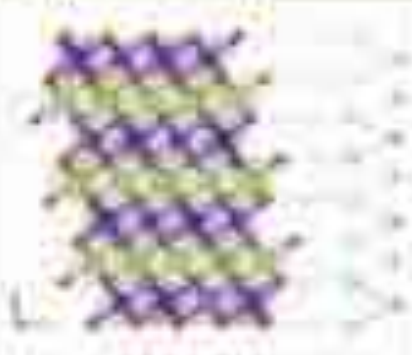
3. Battery recycling using ML-guided electrochemical experiments[7,8,9]

Methods/**software**:

- First-principles calculations (**VASP, CP2K, Orca**)
- AI/ML potentials (**FLARE, Allegro, MACE**)
- Metadynamics (**PLUMED**)
- Electrochemical experiments

Representative publications





CSSE: Center for Scientific Software Engineering

https://ssecenter.cc.gatech.edu/

History: Created in December 2021 as part of Schmidt Futures' $40M Virtual Institute for Scientific Software

Mission:

- CSSE will advance and support scientific research by applying modern software engineering practices, cutting-edge technologies, and modern tools to the development of scientific software within and outside GT
- CSSE will also engage with students and researchers to train the next generation of SW engineering leaders

Team: 4-5 professional software engineers with a combined 50+ years of industry experience

CSSE and ChBE: CSSE can help ChBE researchers with their research projects and research proposals

Vision:

Georgia Tech Software Engineering Center

Georgia Tech College of Computing
Center for Scientific Software Engineering

Open Source Program Office

https://ospo.cc.gatech.edu/ **https://github.com/gt-ospo**

History: Created in August 2023 through a grant from Sloan Foundation

Mission:

- Georgia Tech's Open Source Program Office provides guidance on open source licensing and publication processes and training for topics related to OSS security, AI models, and best practices
- Provides seed funding and summer programs to engage students with open source development for Georgia Tech faculty

Team: 3 part-time faculty with connections to CoC, CSSE, PACE, and GT's Library

OSPO and ChBE: CSSE can help ChBE researchers with their research projects and research proposals

Vision:

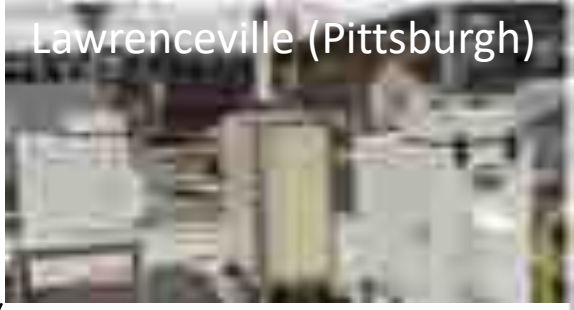
Georgia Tech Software Engineering Center

Georgia Tech College of Computing
Center for Scientific
Software Engineering

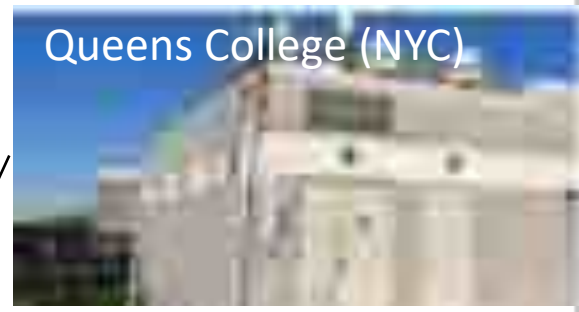
Delta Junction

Yellowstone

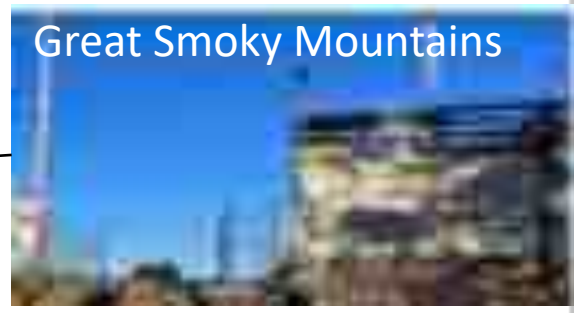
La Casa (Denver)


Lawrenceville (Pittsburgh)

Cheeka Peak/ Makah


Queens College (NYC)

Los Angeles-Pico Rivera

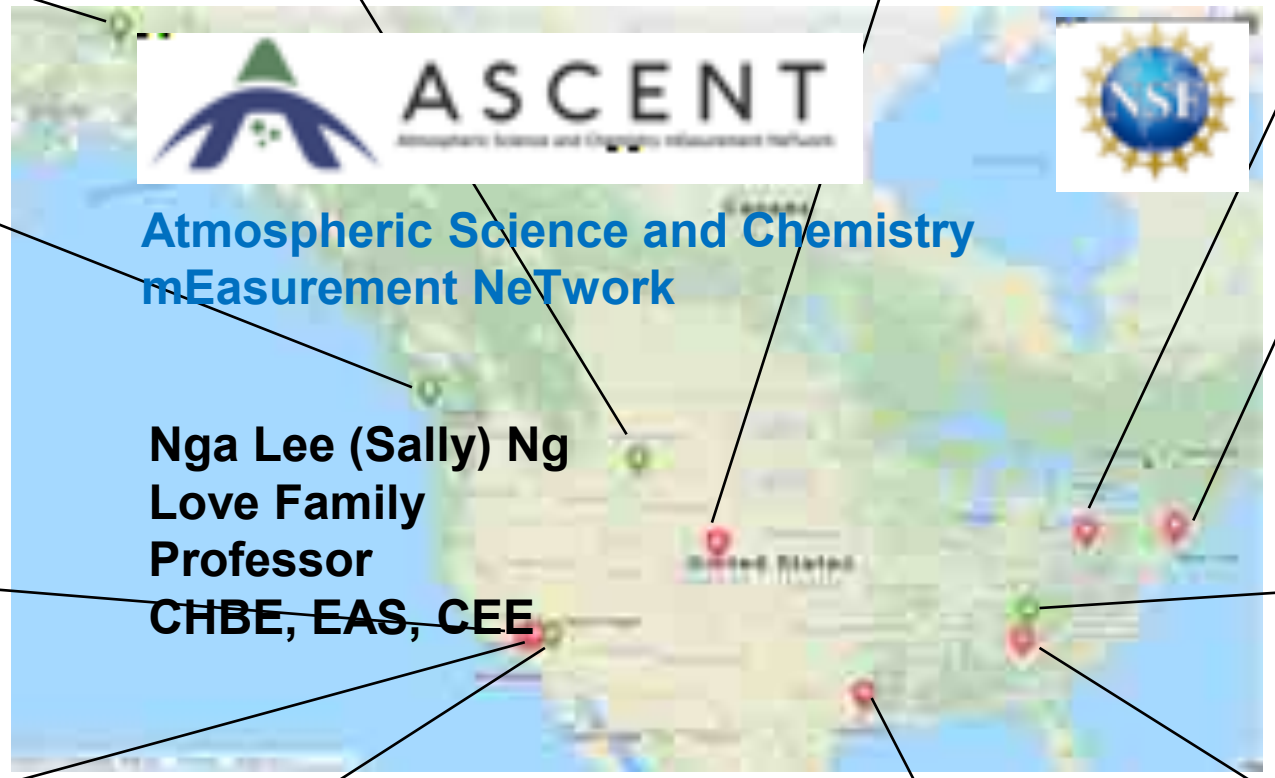

Great Smoky Mountains

Rubidoux (Riverside)

Joshua Tree

Houston

South DeKalb (Atlanta)


ASCENT
Atmospheric Science and Chemistry mEasurement NeTwork
Nga Lee (Sally) Ng
Love Family
Professor
CHBE, EAS, CEE

Yibo Hu

Incoming Assistant Professor @ Illinois Tech

Postdoc @ Georgia Tech

Data Mining, NLP, Trustworthy AI

Efficient & trustworthy data mining methods for societal impact

Passion for cross-disciplinary collaboration.

Intro: AI for Social Dynamics

👤 **Imagine you are a social scientist …**

📍 Track global events

🌍 News overload

❗ Fighting online harms

EU provided Africa economic aid.

.. students planned protests against government..

Georgia Tech College of Computing
Center for Scientific Software Engineering

AI in Cyber: Shared Challenge

👤 Social Scientist → **Cyber Analyst**

🛡️ Detect and stop threats

❌ Misinformation → ✅ Deceive attackers

Global Conflicts

Cyber Threats

AI: Beyond Efficiency

❗ But efficiency is not enough!

❗ Overconfidence is Risky 🚙💥

❓ Can AI know when it does not know?

Conclusion: Research Map

🚀 AI-Driven Applications

- Social Dynamics
- Cybersecurity
- Other Domains…

🔒 Trustworthy AI

- Reliable Classification
- Fair LLMs Generation

Thank You!

Please take a few minutes to give us your feedback here (it’s anonymous):

[CoC + CoE’s ChBE mixer feedback survey]