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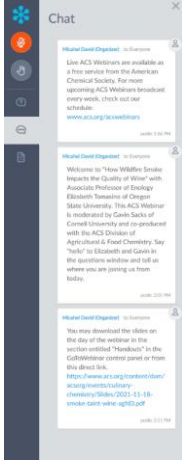


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A Career Planning Tool For Chemical Scientists



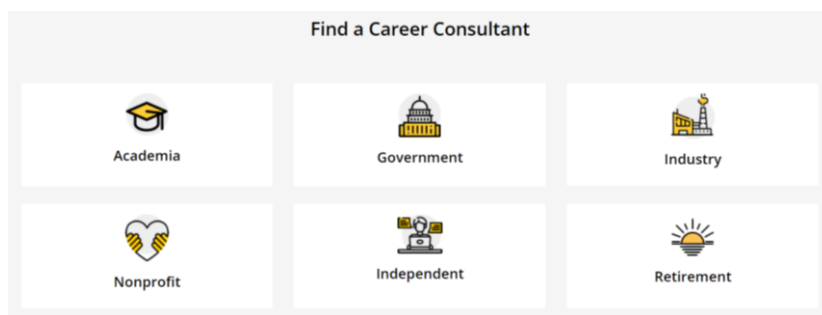
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BS, Massachusetts Institute of Technology, June 2021



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Advancing ACS' Core Value of Diversity, Equity, Inclusion and Respect

Resources

Inclusivity Style Guide

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ACS Webinars on Diversity

Covering diversity and inclusion at the workplace



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Learn more about what Inclusion Moments are and see ideas to host them during your meetings.



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Diversity, Equity, Inclusion, and Respect

**Adapted from definitions from the Ford Foundation Center for Social Justice:

Equity**

Seeks to ensure fair treatment, equality of opportunity, and fairness in access to information and resources for all. We believe this is only possible in an environment built on respect and dignity. Equity requires the identification and elimination of barriers that have prevented the full participation of some groups.

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Inclusion**

Builds a culture of belonging by actively inviting the contribution and participation of all people. Every person's voice adds value, and ACS strives to create balance in the face of power differences. In addition, no one person can or should be called upon to represent an entire community.



Respect

Ensures that each person is treated with professionalism, integrity, and ethics underpinning all interpersonal interactions.

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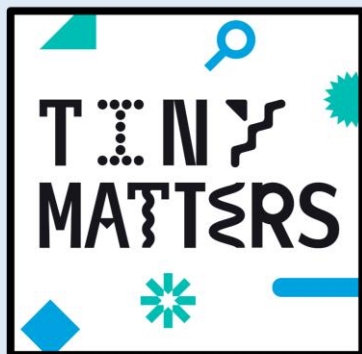
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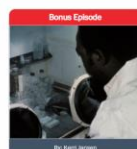
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ACS Career Resources




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Personal Career Consultations



Jim Tung
Marketing
Lacamas Laboratories
B.S., Biochemistry, University of Oregon
Ph.D., Organic Chemistry, University of Notre Dame


Jim Tung works at Lacamas Laboratories in Portland, OR, currently as a business development manager. He has been with Lacamas for 10 years, working on developing new chemical manufacturing projects. Before that, he was a senior research chemist at Obitex Research in Champaign, IL, performing kilo-scale organic chemistry.

An Oregon native, Jim got his B.S. in biochemistry from the University of Oregon, his Ph.D. in organic chemistry from the University of Notre Dame, with postdoctoral experience at Pfizer's laboratories in La Jolla, CA. He is past chair of the Portland Section of the American Chemical Society and was 2019 general co-chair of NCRM 2019. He has interests in process chemistry, labor economics, social media outreach and encouraging career exploration and development for younger chemists.

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AI for Learning, Teaching, and Writing



				
KIRK SCHANZE, PhD	AMY FULLER, PhD	ANDRÉ SILVA PIMENTEL, PhD	ALIVIA ISHEE, PhD	DAMIEN COOPER, BS
Editor-in-Chief, <i>ACS Applied Materials & Interfaces</i> , Chemistry Chair and Professor, University of Texas at San Antonio	Assistant Professor, Chemistry, University of Hawaii-Manoa	Chemistry Associate Professor and Graduate Coordinator, Pontifícia Universidade Católica do Rio de Janeiro	Student Liaison, ACS Undergraduate Student Advisory Board and Fulbright Student Researcher, University of Heidelberg	Student Liaison, ACS Undergraduate Student Advisory Board and Chemistry Student, University of Southern Mississippi

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Poll #1:

Which best describes you?



- Undergrad
- Grad Student
- Educator
- Researcher
- Manager or administrator
- Self-identify (in chat)

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Poll #2:

How do you feel about artificial intelligence tools like ChatGPT?



- Love them! So excited for the next version!
- They are cool but creepy...
- Eh, still undecided
- Still trying to figure out what they are

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Artificial Intelligence the ability of computers to simulate human thought (i.e. ability to problem solve and adapt)

Machine Learning computational tools that function without explicit programming

Deep Learning computational tools designed to function as a human brain

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Emerging AI Tools

- **ChatGPT:** Natural Language Processing (NLP) program trained on data sets of curated webpages, books, and articles
- See also: YouChat, Open AI Playground, Perplexity, Elicit, Google BARD
- **Wolfram|Alpha:** Computational knowledge engine predominantly used to solve complex math and physics equations
- **Fotor:** Image generation program that can produce images in a variety of artistic styles given a prompt

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Poll #3:

Which best describes how you primarily use artificial intelligence tools like ChatGPT?

- Conducting research for work or class
- Finding data or getting ideas for papers or test questions
- Playing around when I'm bored
- I have a PDA that gets my voice commands wrong. Does that count?



Enter other uses in chat

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What's Next?

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Panelist

Amy Fuller, PhD

Assistant Professor of Chemistry
University of Hawaii-Manoa

"Potential ChatGPT Use in Undergraduate Chemistry Laboratories"
Tim Humphry and Amy L. Fuller
Journal of Chemical Education 2023 100 (4), 1434-1436
DOI: 10.1021/acs.jchemed.3c00006

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Should I use AI?

HELP ME GET STARTED ON AN ASSIGNMENT

HELP ME IMPROVE ON WHAT I'VE ALREADY DONE

EXPLAIN AN IDEA IN SIMPLER TERMS OR IN A DIFFERENT WAY

FULLY COMPLETE AN ASSIGNMENT FOR ME

HELP WITH MY RESEARCH AND FIND FACTS, QUOTES OR RESOURCES

YES

NO

<https://www.aiforeducation.io/>

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Prompt Engineering Chat-GPT 3.5 (free)

- Give Chat-GPT its character
- Include a lot of details for what you want
- Try again
- **Tips:** History on or off?
 - Double check all information

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Panelist

André Silva Pimentel, PhD

Chemistry Associate Professor and Graduate
Coordinator
Pontifícia Universidade Católica do Rio de Janeiro

"Do Large Language Models Understand Chemistry? A
Conversation with ChatGPT"

Cayque Monteiro Castro Nascimento and André Silva
Pimentel

Journal of Chemical Information and Modeling. 2023 63 (6),
1649-1655

DOI: 10.1021/acs.jcim.3c00285



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What do AI systems know?

Chemical representation

Name	SMILES
Ethane	C=C
Propane	C(C)(C)C
Pentane	CCCCC

ChatGPT ~27%
(Mar 23)

BARD ~100%
(Jul 14)

35

What do AI systems know?

Chemical representation

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Ethane	C=C
Propane	C(C)(C)C
Pentane	CCCCC

ChatGPT ~27%
(Mar 23)

BARD ~100%
(Jul 14)

Hydrophobicity

Name	LogP _{ChatGPT}	% error
limonene	4.7	7
γ-terpinene	4.2	-4
eugenol	4.6	106

ChatGPT ~31%
(Mar 23)

BARD << error,
but wrong
explanations

36

What do AI systems know?

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ChatGPT ~31%
(Mar 23)

BARD << error,
but wrong
explanations

Coordination compound geometry

Name	Geometry	Correct?
[Ag(NH ₃) ₂] ⁺	Linear	Yes
CoCl ₂ (pyr) ₂	Square planar	No (tet)
[Cu(CN) ₃] ²⁺	Trigonal planar	Yes

ChatGPT ~58%
(Mar 23)

BARD ~100%
(Jul 14)

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What do AI systems know?

Chemical representation

Name	SMILES
Ethane	C=C
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ChatGPT ~27%
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BARD ~100%
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[Cu(CN) ₃] ²⁺	Trigonal planar	Yes

ChatGPT ~58%
(Mar 23)

BARD ~100%
(Jul 14)

Point groups & Symmetry

Molecule	Point group	Correct?
H ₂ O	C _{2v}	Yes
CH ₄	C _{3v}	No, (T _d)
Ferrocene	D _{5h}	Yes

ChatGPT ~60%
(Mar 23)

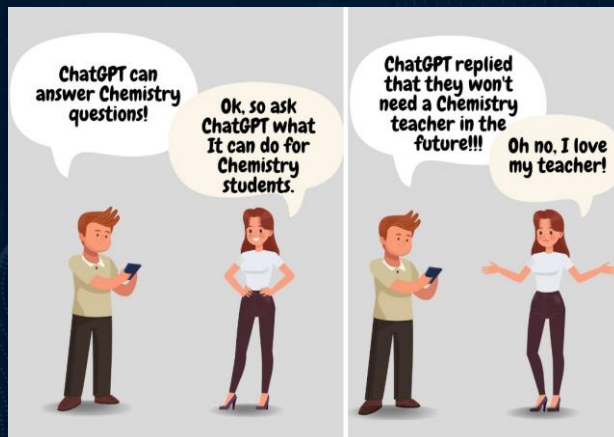
BARD ~100%
(Jul 14)

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The hope... or more fear?



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Panelist
Kirk S. Schanze, PhD

Robert A. Welch Professor, Chemistry
 Department, University of Texas at San Antonio
 Editor-in-Chief
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"Best Practices for Using AI When Writing Scientific
 Manuscripts Caution, Care, and Consideration: Creative
 Science Depends on It"
 Jillian M. Buriak, et al
 ACS Nano 2023 17 (5), 4091-4093
 DOI: 10.1021/acsnano.3c01544

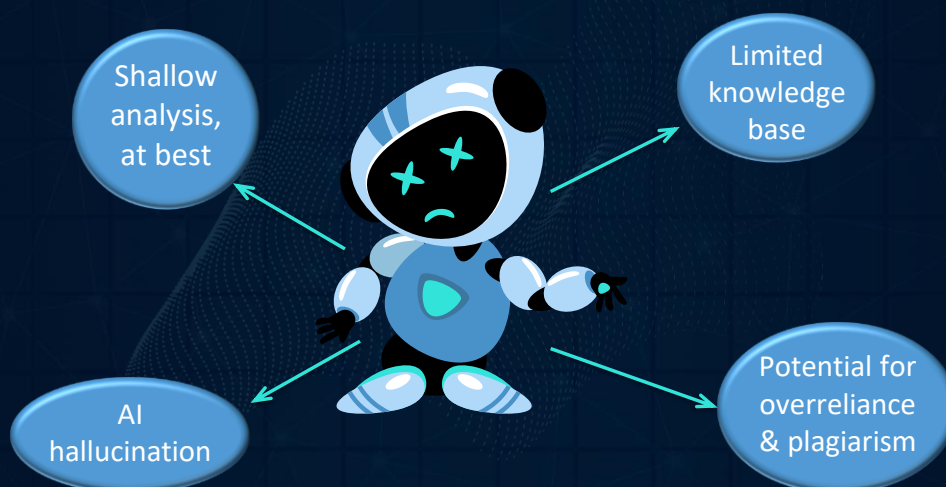
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Scientific Communication: AI Strengths and Benefits



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Scientific Communication: AI Cautions and Concerns



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Summary Recommendations

- No cut & paste
- Treat ChatGPT output as very early draft
- Verify citations
- Acknowledge, in the Acknowledgments and Experimental Sections, your use of an AI bot/ChatGPT
 - Do **not** list as co-author



Reproduced from: ACS Energy Letters 2023, 8, 1, 878–880

Use ChatGPT to expand your horizons & spark new ideas, not replace your own creativity!

Scientific Communication: Lead References

- AI et al.: Machines Are About to Change Scientific Publishing Forever, Gianluca Grimaldi and Bruno Ehrler, ACS Energy Letters 2023 8 (1), 878-880, DOI: 10.1021/acseenergylett.2c02828
- Best Practices for Using AI When Writing Scientific Manuscripts Caution, Care, and Consideration: Creative Science Depends on It, Jillian M. Buriak, et al. ACS Nano 2023 17 (5), 4091-4093, DOI: 10.1021/acsnano.3c01544
- Was This Title Generated by ChatGPT? Considerations for Artificial Intelligence Text-Generation Software Programs for Chemists and Chemistry Educators, Mary E. Emenike and Bright U. Emenike, Journal of Chemical Education 2023 100 (4), 1413-1418, DOI: 10.1021/acs.jchemed.3c00063

Let's Chat!



Amy Fuller, PhD
Assistant Professor of Chemistry
University of Hawaii - Manoa



André Silva Pimentel, PhD
Chemistry Associate Professor and
Graduate Coordinator
Pontificia Universidade Católica do Rio de
Janeiro



Kirk Schnaze, PhD
Editor - in - Chief
ACS Applied Materials and Interfaces

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Will AI Win a Chemistry Nobel Prize and Replace Us?

Prof. Jeremy Frey
Computational Systems Chemistry,
School of Chemistry
University of Southampton



Expanding the Role of Machine Learning in Chemistry

Dr. John Jumper
Google DeepMind
London, United Kingdom



What Artificial Intelligence Can Do to Accelerate Chemical Discovery

Prof. Heather Kulik
Department of Chemical Engineering
Massachusetts Institute of Technology

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Poll #2 (Revisited):

How do you feel about artificial intelligence tools like ChatGPT?


- Love them! So excited for the next version!
- They are cool but creepy...
- Eh, still undecided
- Still trying to figure out what they are



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Mike Russell Erik

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