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Chat

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BS, Massachusetts Institute of Technology, June 2021

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- Quick Guide: How to host inclusive in-person events

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Jim Tang
Research
Organic Chemistry
UCL, Chemistry, University of London

Jim Tang works at Unilever Laboratories in Hertfordshire, UK, currently as a senior drives manager. He has been with Unilever for 10 years, working on developing new chemical reaction projects. Before that, he was a senior technical specialist within the Innovation Research in Campinas, Brazil, working on new and novel products.

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AI for Learning, Teaching, and Writing

KIRK SCHANZE, PhD
Editor-in-Chief, ACS Applied Materials & Interfaces, Chemistry Chair and Professor, University of Texas at San Antonio

AMY FULLER, PhD
Assistant Professor, Chemistry, University of Hawaii–Manoa

ANDRÉ SILVA PIMENTEL, PhD
Chemistry Associate Professor and Graduate Coordinator, Pontifícia Universidade Católica do Rio de Janeiro

ALIVIA ISHEE, PhD
Student Liaison, ACS Undergraduate Student Advisory Board and Fulbright Student Researcher, University of Heidelberg

DAMIEN COOPER, BS
Student Liaison, ACS Undergraduate Student Advisory Board and Chemistry Student, University of Southern Mississippi

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Artificial Intelligence for learning, teaching, and writing

ACS Webinars
August 10, 2023

Moderators

Damien Cooper
University of Mississippi

Alivia Ishee
University of Florida

2023 Student Liaisons, ACS Undergraduate Student Advisory Board
Poll #1:
Which best describes you?
- Undergrad
- Grad Student
- Educator
- Researcher
- Manager or administrator
- Self-identify (in chat)

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
**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

---

**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
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

What’s Next?
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

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/
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

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
### Chemical representation

<table>
<thead>
<tr>
<th>Name</th>
<th>SMILES</th>
<th>ChatGPT ~27% (Mar 23)</th>
<th>BARD ~100% (Jul 14)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ethane</td>
<td>C=C</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Propane</td>
<td>C(C)(C)C</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Pentane</td>
<td>CCCCC</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### Hydrophobicity

<table>
<thead>
<tr>
<th>Name</th>
<th>LogP&lt;sub&gt;ChatGPT&lt;/sub&gt;</th>
<th>% error</th>
</tr>
</thead>
<tbody>
<tr>
<td>limonene</td>
<td>4.7</td>
<td>7</td>
</tr>
<tr>
<td>γ-terpinene</td>
<td>4.2</td>
<td>-4</td>
</tr>
<tr>
<td>eugenol</td>
<td>4.6</td>
<td>106</td>
</tr>
</tbody>
</table>

ChatGPT ~31% (Mar 23)  
BARD << error, but wrong explanations
### What do AI systems know?

#### Chemical representation

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<td>eugenol</td>
<td>4.6</td>
<td>106</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

#### Coordination compound geometry

<table>
<thead>
<tr>
<th>Name</th>
<th>Geometry</th>
<th>Correct?</th>
<th>ChatGPT</th>
<th>BARD</th>
</tr>
</thead>
<tbody>
<tr>
<td>[Ag(NH₃)₂]⁺</td>
<td>Linear</td>
<td>Yes</td>
<td>~58%</td>
<td>~100%</td>
</tr>
<tr>
<td>CoCl₂(pyr)₂</td>
<td>Square planar</td>
<td>No (tet)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>[Cu(CN)₃]²⁻</td>
<td>Trigonal planar</td>
<td>Yes</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

#### Point groups & Symmetry

<table>
<thead>
<tr>
<th>Molecule</th>
<th>Point group</th>
<th>Correct?</th>
<th>ChatGPT</th>
<th>BARD</th>
</tr>
</thead>
<tbody>
<tr>
<td>H₂O</td>
<td>C₂ᵥ</td>
<td>Yes</td>
<td>~60%</td>
<td>~100%</td>
</tr>
<tr>
<td>CH₄</td>
<td>C₃ᵥ</td>
<td>No, (T₅)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ferrocene</td>
<td>D₉h</td>
<td>Yes</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
The hope… or more fear?

ChatGPT can answer Chemistry questions!

Ok, so ask ChatGPT what it can do for Chemistry students.

ChatGPT replied that they won’t need a Chemistry teacher in the future!!!

Oh no, I love my teacher!

Panelist
Kirk S. Schanze, PhD

Robert A. Welch Professor, Chemistry Department, University of Texas at San Antonio
Editor-in-Chief
ACS Applied Materials and Interfaces
ACS Applied Materials Family Journals

*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
Scientific Communication: AI Strengths and Benefits

- Jump-start your writing
- Level the playing field
- Refine your text
- Highlight overlooked topics

Scientific Communication: AI Cautions and Concerns

- Shallow analysis, at best
- Limited knowledge base
- AI hallucination
- Potential for overreliance & plagiarism
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

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

Scientific Communication: Lead References

- 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
Pontifícia Universidade Católica do Rio de Janeiro

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

Plenary Session: Harnessing the Power of Data
Sunday, August 13 | 5:00 PM - 7:00 PM PT | Room 24/25, Moscone Center, South

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
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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