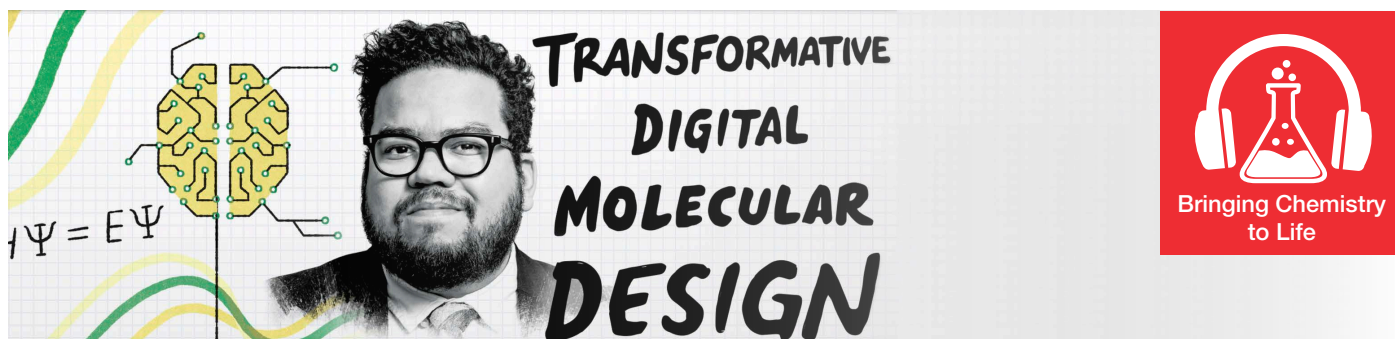


# Bringing Chemistry to Life podcast series

ThermoFisher  
SCIENTIFIC

Season 4: **Expanding Chemistry Perspectives**  
Episode 3: **Chemistry, Computers and Humans**



## Episode abstract

This started with a TV in the background showing Brazil playing Croatia in the World Cup quarter-finals, and ended up with Brazil's surprising defeat, for the dismay of our guest, Brazil-born Gabe Gomes. In the middle, the most approachable conversation you'll ever hear about computational chemistry.

Gabe tries to solve real world problems using computers and it's almost a paradox that such an extrovert, fun guy, in love with music and speaking so much about people, ends up investing his life in machine learning algorithms. And yet it takes courage and creativity to dare going in new directions and seeking the next big problem at the interface of scientific disciplines.

Chemistry is a complex multivariate problem and resolving this complexity is the key to the fundamental understanding we need to advance the discipline. Gabe is a wonderful chaperone in our journey to discover how automation and optimization can be used not to replace chemists, but to free them to apply their skills where it matters the most. And he is the living demonstration that computers and humans can be part of the same discourse.

## About our guest

### Gabe Gomes, PhD

Assistant Professor, Department of Chemistry and Department of Chemical Engineering, Carnegie Mellon University

Gabe's group site: <https://www.gpggrp.com>

## Gabe's Recent Publications:

- [Navigating through the Maze of Homogeneous Catalyst Design with Machine Learning](#)
- [A comprehensive discover platform for organophosphorus ligands for catalysis](#)
- [Stereolectronics-aware molecular representation learning](#)

## Gabe's Content Recommendations:

- [The Code Breaker: Jennifer Doudna, Gene Editing, and the Future of the Human Race](#), a book by Walter Isaacson
- [In Rainbows](#), a live performance by Radiohead.
- [Mr. Robot](#), a television show by Sam Esmail
- [Blade Runner 2049](#), a movie by Denis Villeneuve
- [Watchmen](#), a series by Damon Lindelof and the Original Soundtrack for [Watchmen](#) by Trent Reznor and Atticus Ross

This podcast series is available via the following links



Products are processed under ISO 9001:2015 quality management systems and samples are tested for conformance to the noted specifications. Certain data may have been supplied by third parties. We disclaim the implied warranties of merchantability and fitness for a particular purpose, and the accuracy of third party data or information associated with the product. Products are for research and development use only. Products are not for direct administration to humans or animals. It is the responsibility of the final formulator or end user to determine suitability, and to qualify and/or validate each product for its intended use. © 2023 Thermo Fisher Scientific Inc. All trademarks are the property of Thermo Fisher Scientific and its subsidiaries unless otherwise specified. **01\_2023**

thermo scientific