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 in 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
• Stereoelectronics-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 Aticus Ross

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