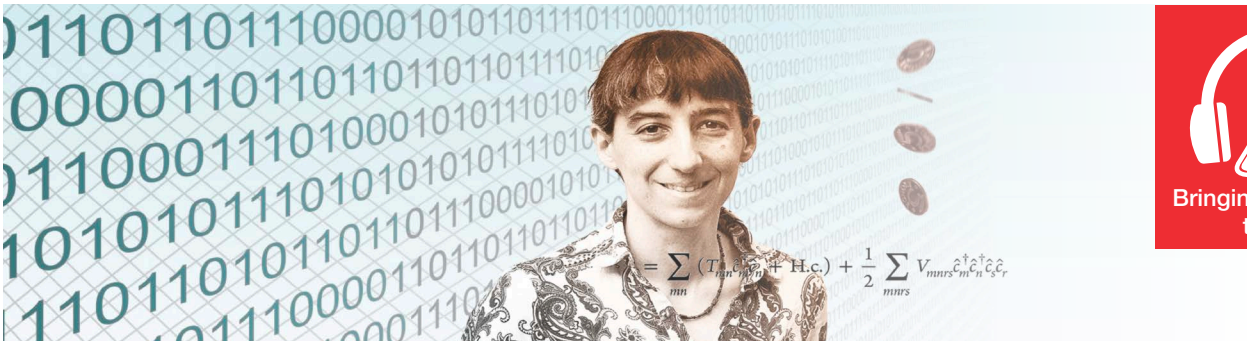
Bringing Chemistry to Life podcast series

Thermo Fisher SCIENTIFIC

Season 1: **The 2019 C&EN's Talented 12**
Episode 8: **Chemical computers and other tales from a chemical mind**



Bringing Chemistry to Life

Episode abstract

Theoretical chemistry is one of those subjects that can intimidate even the most passionate experimental chemist. Complex theories rooted in super-advanced mathematics to model a chemical bond length are not everyone's cup of tea. Yet it does not have to be like that and it takes brilliant minds like Brenda Rubenstein's to make it so elegantly obvious. Brenda and Paolo's discussion is as approachable as it gets; a surprisingly eye-opening discovery of how theory can have profound effects on experimental practice. Brenda talks through her efforts in finding the right balance between molecular simulations' theoretical rigor and their practical utility, and opening the door to her incredible creative thinking and courage in pursuing disruptive ideas. Her novel paradigm for the computer of the future, where chemistry is used to achieve massive increases in data storage density compared to traditional semiconductor technologies, represents truly out-of-the-box. As if all this wasn't enough, we also find a brilliant example of social responsibility in Brenda's commitment to change lives of children from low-income background through facilitating access to STEM education. An unmissable episode.

About our guest

Brenda M. Rubenstein, PhD

Joukowsky Family Assistant Professor of Chemistry, Brown University

Brenda's group site:
https://www.brown.edu/research/labs/rubenstein/home

C&EN Talented 12 profile of Brenda:
https://cen.acs.org/physical-chemistry/theoretical-chemistry/Brenda-Rubenstein/97/i33

Recent Publications from Brenda:

- Predicting the Viability of Beta-Lactamase: How Folding and Binding Free Energies Correlate with Beta-Lactamase Fitness
- Multicomponent molecular memory
- Encoding Information in Synthetic Metabolomes
- Molecular data storage
- *Ab initio* Finite Temperature Auxiliary Field Quantum Monte Carlo
- Observation of a π-Type Dipole-Bound State in Molecular Anions

Brenda's Content Recommendations:

- Statistical Mechanics of Deep Learning (a paper by Bahri, et al. on machine learning)
- The Thermodynamics of Computation – A Review (a review article by Charles H. Bennett)
- Where is the Land of Opportunity? (a paper Chetty, et al. on intergenerational mobility)
- Alterlife and Decolonial Chemical Relations (a Cultural Anthropology article by Michelle Murphy)

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