Benjamin Sanchez-Lengeling

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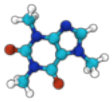

Education

'14-'19 **PhD candidate in Chemistry and Chemical Biology**, *Harvard University*, USA.

- Secondary Field in Computational Science and Engineering (CSE).
- Graduate Consortium on Energy and Environment.

Scholarship awardee by the Chemistry and Chemical Biology Department. My adviser is Alán Aspuru-Guzik.

'11-'13 **European Master in Theorethical Chemistry and Computational Modelling**, *University of Valencia (UV)* , Spain.
2 year Erasmus Mundus scholarship awardee by the European Union.

'05-'11 **Bachelor's Degree in 1) Mathematics and 2) Computer Science**, *University of Guanajuato (UG)*, Mexico.
Scholarship awardee by the Centro en Investigacion en Mathematicas (CIMAT) for 9 semesters.

Research focus

My research centers around using machine learning techniques to 1) build data-driven models for prediction of molecular properties and 2) generation of new molecules and materials via generative models. Prominent work includes:

- Inverse molecular design using machine learning: Generative models for matter engineering, Science, '18, 10.1126/science.aat2663
- Automatic chemical design using a data-driven continuous representation of molecules ACS Central Science, '18, arXiv:10.1021/acscentsci.7b00572.
- Objective-reinforced generative adversarial networks (ORGAN) for sequence generation models, '17 arXiv:1705.10843.
- Design Principles and Top Non-Fullerene Acceptor Candidates for Organic Photovoltaics Joule, '17, 10.1016/j.joule.2017.10.006

Google Scholar link: https://scholar.google.com/citations?user=-91dFcMAAAAJ&hl=en.

Clubes de Ciencia Mexico and Science Clubs Internacional

Role ***Founding Member, Technology Operations director. Board member of Science Clubs International***

Time '14-Current

Websites clubesdeciencia.mx, clubesdeciencia.org

About Clubes de Ciencia Mexico is a growing organization of young scientist in the US and Mexico dedicating to Science education. Our program has been implemented in five editions, amounting to more than 200 different clubs, imparted by 400 instructors from all around the world and more than 3200 participating students. We have received more than 500k dollars in funding from grants, organizations and private donors. I have worked in many aspects of the organization. Currently managing a group of volunteers and programmers that work on automating and implementing efficient applications that can handle the tasks and logistics of our organization. Science Clubs International is an organization that coordinates efforts of 7 countries on implementing the "Science Clubs" program.

RIIAA: Reunión Internacional de Inteligencia Artificial y sus Aplicaciones

Role ***Founding Member, Organizer***

Time ’18-Current

Website riiaa.org

About RIIAA is an international conference for artificial intelligence and its applications, RIIAA intends to create a meeting point for academics, researchers, industry, and government in Mexico and Latin-America. We organized the first edition this past August 2018 with around 250 attendees from all sectors. I imparted a day-long summer school as an introduction to deep learning. Work for this event involved working in a team with other organizers, planning logistics of the conference, searching for funding (Deepmind and Facebook) and securing speakers.

Work and teaching experience

Workshops I have developed several workshops on applied science; these workshops tend to be a week-long, around 6 hours a day and catered to a group of 20 to 80 people. I have implemented these workshops along with local organizations that focus on scientific education in Mexico, Spain, UK and the US, the *algorave* music tour (’12-’13) and *clubes de ciencia* programs (’14-’18). Topics include programming physical systems, the creation of generative art, live-coding, energy policy, machine learning, deep learning, and quantum chemistry.

Oct ’18-Mar ’19 **Intern**, *Google*, USA.
Worked with the nosebrain team at Google Brain in Cambridge, MA.

Mar-Dic ’17 **Teaching Fellow for QuantumWorldX**, *Harvard University*, USA.
HarvardX massive open online course around Quantum Mechanics and Chemistry. Course had more than 6000 students, I designed the programming aspect of the course and would answer questions in the course forums.

Aug-Dic ’16 **Teaching Fellow for Chem160**, *Harvard University*, USA.
Course was a introduction to Quantum Mechanics in a Chemical setting. Was awarded a **Certificate of Teaching Excellence** for my work in the course.

Jan - May ’15 **Lab Teaching Fellow for PS10**, *Harvard University*, USA.
Managed 4 laboratory sections, 20 students each for an introductory physical chemistry course.

Sept ’13 - Jan ’14 **Affiliate Scholar**, *College of Chemistry, UC Berkeley*, USA.
Participated in Professor William Lester Jr’s group working with applications of Quantum Monte Carlo (QMC) to CH+Acrolein reactions and on a efficient zero time-step extrapolation algorithm.

Sept ’13 - Jul ’14 **Research Engineer**, *Laboratoire de Chimie et Physique Quantiques, Université Paul Sabatier* , Toulouse , France.
Employee for Michel Caffarel’s group, working on surveying various QMC codes, doing research on magnetic couplings for organic compounds, trying to port algorithms to a GPU platform.

Feb - Sept ’11 **Consultant**, *Industrial Mathematics group, CIMAT*, Guanajuato.
Worked in Dr. Noberto Flores’s group implementing a C++ toolbox for oil reservoir characterization, which included visualization methods and seismic signal processing algorithms. This project was a collaboration between CIMAT and PEMEX.

Feb - Dic ’08 **Research Assistant**, *Music Department*, University of Guanajuato, Mexico.
Worked for Dr. Roberto Morales Manzanares, as a mathematics and programming assistant, aiding in data collection and analysis for real time gesture recognition and musical enhancement.

Computer skills

Languages Python, C, C++, CUDA, Fortran, Java, Matlab, R, Supercollider (Smalltalk) and Processing.

Libraries Tensorflow, Keras, Pytorch, Scientific Python, pandas, RDKit, Openbabel