

# Designing the Materials for the Sustainable Age of Humanity



Alán Aspuru-Guzik  
Professor, Chemistry and Chemical Biology

## CURRENT RESEARCH

### Developing computer programs for simulating molecules exactly using quantum computers

Professor Alán Aspuru-Guzik seeks to make a difference in facing the most important challenge of the 21st century, namely the transition to a renewable energy economy. One of the key aspects that holds us back is the current slow and painful cycle of materials discovery. Alán is a pioneer in the emerging area of materials genomics: He uses a powerful combination of millions of quantum chemical calculations, state-of-the-art machine learning algorithms and big data techniques to sift through millions and millions of candidate molecules in search of the next generation of materials. He works with experimental groups around the world to collaborate in a virtuous cycle of computational design and experimental synthesis and characterization that promises to accelerate materials discovery by a factor of ten. Alán focuses on the discovery of inexpensive organic solar cells that could help provide power to the 1.4 billion people that lack access to the electrical grid. He works in the development of all-organic flow batteries for large-scale energy storage that promise to free the world from fossil fuels. He also works in the development of organic light-emitting diodes that could help provide efficient and inexpensive lighting sources with innovative form factors.

In another line of research, Professor Alán Aspuru-Guzik wants to go beyond the use of traditional or *classical* computers. These computers, which range from your cell phone to the largest supercomputers in the world, cannot simulate molecules and materials exactly. A new promising class of computers, *quantum* computers, enable the exact simulation of molecules and materials. Alán is a pioneer in the development of algorithms for these computers to simulate materials and in collaborating with experimental groups around the world to implement them.

Working at the interface of theoretical chemistry and other fields, in particular computer science, applied mathematics, and...

## AFFILIATION

Harvard University

## EDUCATION

- Ph.D., in Chemistry, 2004 , University of California, Berkeley ,

## AWARDS

- 2013 ACS Early Career Award in Theoretical Chemistry
- 2010 MIT Technology Review Young Innovator Under 35 (TR35)
- 2009 DARPA Young Faculty Award
- 2009 Camille and Henry Dreyfus Teacher-Scholar
- 2009 Sloan Research Fellow

## RESEARCH AREAS

- Environment
- Chemical
- Computational Sciences / Mathematics
- Materials Science / Physics

## FUNDING REQUEST

Your contributions will support the continued research of Professor Alan Aspuru-Guzik, of Harvard University, as he works to design the best materials for important energy applications using computers. Your donations will fund the necessary \$150K/year for each project required to work on these new directions not currently funded by federal agencies. In choosing to donate, you will play a role in exploring the development of novel molecules for solar-thermal renewable energy plants, the development of green and clear insulators for energy distribution, exploring the use of our technology in novel anti-bacterial molecules, and also in the development of photodynamic therapy molecules for targeting cancer.

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