center for excitonics

Finding renewable energy materials using one screensaver at a time: Combinatorial quantum chemistry for organic photovoltaics

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Abstract: During this talk, I will describe our group's efforts in the Clean Energy Project (http://cleanenergy.harvard.edu) , a collaboration with the IBM World Community Grid to search for novel materials for organic photovoltaics and organic electronics using computational resources from volunteer donors around the world. Our project aims to find new materials using techniques from ab initio quantum chemistry combined with cheminformatics tools that are usually employed for the discovery of novel pharmaceutical compounds. To date, we have computed more than five million structures using first-principles methods, and have analyzed three million using cheminformatics. I will describe our progress so far, and describe immediate goals. A computationally-predicted material with an unusally high hole mobilty of 13 cm^2/Vs was synthesized by Zhenan Bao's group at Stanford. I will describe this experimental collaboration as well.

Bio Alán Aspuru-Guzik received his undergraduate degree in Chemistry from the National Autonomous University of Mexico (UNAM) in 1999. He received the Gabino Barreda Medal from UNAM, which prizes the top achiever in each field of study. After receiving his PhD in Physical Chemistry from the University of California, Berkeley in 2004, under Professor William A. Lester, Jr., he was a postdoctoral scholar in the group of Martin Head-Gordon at UC Berkeley from 2005-2006.

Professor Aspuru-Guzik carries out research at the interface of quantum information and chemistry. In particular, he is interested in the use of quantum computers and dedicated quantum simulators for chemical systems. He has studied the role of quantum coherence in excitonic energy transfer in photosynthetic complexes, and developed methodology for studying the spectroscopy of molecules in nanoscale environments. He and his group recently developed a density functional theory for open quantum systems. He leads the Clean Energy Project: a distributed computing effort for screening renewable energy materials.

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