Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

The Harvard Clean Energy Project: High-throughput screening of organic photovoltaic materials using first-principles electronic structure theory JOHANNES HACHMANN, ROBERTO OLIVARES-AMAYA, SULE ATAHAN-EVRENK, Harvard University, CARLOS AMADOR-BEDOLLA, Universidad Nacional Autonoma de Mexico, ALAN ASPURU-GUZIK, Harvard University — We present the Harvard Clean Energy Project (CEP) which is concerned with the computational screening and design of new organic photovoltaic materials. CEP has established an automated, high-throughput, in silico framework to study millions of potential candidate structures. This presentation discusses the CEP branch which employs first-principles computational quantum chemistry for the characterization of molecular motifs and the assessment of their quality with respect to applications as electronic materials. In addition to finding specific structures with certain properties, it is the goal of CEP to illuminate and understand the structure-property relations in the domain of organic electronics. Such insights can open the door to a rational, systematic, and accelerated development of future high-performance materials. CEP is a large-scale investigation which utilizes the massive computational resource of IBM's World Community Grid. In this context, it is deployed as a screensaver application harvesting idle computing time on donor machines. This cyberinfrastructure paradigm has already allowed us to characterize 3.5 million molecules of interest in about 50 million DFT calculations.

Johannes Hachmann
Harvard University

Date submitted: 08 Dec 2011 Electronic form version 1.4