Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

The Harvard Clean Energy Project. Large-scale computational screening and design of molecular motifs for organic photovoltaics on the World Community Grid JOHANNES HACHMANN, ROBERTO OLIVARES-AMAYA, SULE ATAHAN-EVRENK, Harvard University, CARLOS AMADOR-BEDOLLA, UNAM Mexico, ALAN ASPURU-GUZIK, Harvard University — Organic solar cells are one of the promising approaches to ubiquitously establishing renewable energy sources; alas the necessary 10% energy conversion efficiency remains elusive. We present the Harvard Clean Energy Project (CEP, http://cleanenergy.harvard.edu) which is concerned with the screening and design of organic photovoltaics (and organic electronics in general) by means of first-principles computational quantum chemistry. We use modern DFT to assess the quality of candidate structures and systematically improve upon these based on the gathered understanding of structure-property relations. The CEP is a high-throughput investigation which utilizes the massive computational resource of the IBM World Community Grid, which allows us to characterize millions molecules of interest in the course of the next year. We address the combinatorial generation of our molecular library, our database, workflow organization and automation, data calibration and cheminformatics analysis, and the closure of the development cycle provided by our experimental collaborators.

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Date submitted: 29 Nov 2010 Electronic form version 1.4