Harvard Clean Energy Project (CEP)

We are living in the age of energy. The fossil fuel based economy of the present must give way to the renewable energy based economy of the future. Getting there is the grandest challenge humanity faces. Chemistry can help meet this challenge by discovering new materials that efficiently harvest solar radiation, store energy for later use, and reconvert the stored energy when needed.

The Clean Energy project uses computational chemistry, the support of IBM's World Community Grid and the willingness of people to help look for the best molecules possible for: organic photovoltaics to provide inexpensive solar cells, polymers for the membranes used in fuel cells for electricity generation, and how best to assemble the molecules to make those devices.

The current project phase is concerned with the characterization of millions of molecular motifs using first-principles quantum chemistry. The scale of this study requires a correspondingly large computational resource, which is provided by distributed volunteer computing on IBM’s World Community Grid. The results are compiled and analyzed in an extensive reference database and
will be made available for public use. In addition to finding specific candidates 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 and systematic design of future high-performance materials. The computational work in CEP is tightly embedded in a collaboration with experimentalists, who provide valuable input and feedback to the project.

Thanks to all the generous help from volunteers like you, we have by now collected 10 million unique results in 12,500 years of computing time. The former corresponds to 120 million individual density functional theory calculations - which is a rather incredible number. It is most likely of the same order of magnitude as all quantum chemistry calculations that have been run in the history of quantum chemistry!

You can also contribute to this effort. Click the link below to download our screen-saver:

http://www.worldcommunitygrid.org/reg/viewRegister.do

You can also follow us on our facebook page to receive regular updates: