# WORLD COMMUNITY GRID


Grid Computing and Energy

www.worldcommunitygrid.org

# How „grid computing“ works

**Grid Computing: The Basics**
Grid computing joins together many individual computers, creating a large system with massive computational power that far surpasses the power of a handful of supercomputers.

**Changing Our World Now**
Grid computing is not futuristic, it is only at work and can be used in projects which benefit all of us.

Our first project, Human Proteome Folding, is identifying the proteins produced by human genes. With this information, scientists can understand how defects in proteins can cause disease, making it easier to find cures. 44 potential treatments were found within less than three months, without grid computing, it would have taken more than one year.

# The clean energy project

**Mission**

The mission of the Clean Energy Project is to find new materials for the next generation of solar cells and later, energy storage devices. By harnessing the immense power of World Community Grid, researchers can calculate the electronic properties of tens of thousands of organic materials – many more than could ever be tested in a lab – and determine which candidates are most promising for developing affordable solar energy technology.

**Significance**

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, but getting there is the greatest challenge humanity faces. With the help of chemistry we are able to find new ressources and progress in that way.

**Approach**

Researchers are employing molecular mechanics and electronic structure calculations to predict the optical and transport properties of molecules that could become the next generation of solar cell materials.

a) Molecular mechanics calculations: Some of the computers contributing to the Clean Energy Project are carrying out molecular mechanics calculations of molecular crystals, thin films and molecular and polymer blends to study the packing arrangements and for predicting charge and excitation energy transport properties of the candidate materials.

These calculations will be carried out using the CHARMM molecular mechanics package developed by the Karplus group at Harvard University.

b) Electronic structure calculations: To obtain the relevant optical and electronic transport properties, some of the computers connected to the Clean Energy Project will be computing calculations using wave function methods (such as Hartree-Fock or second-order perturbation theory) and density functional theory.

These calculations will help researchers build a database of molecular properties that together with the results of the molecular mechanics calculations will help us identify potential candidate materials. The electronic structure calculations will be performed with the Q-Chem quantum chemistry code, developed by Q-Chem, Inc.