If you don't try, you'll never know

Timothy Clark

Computer-Chemie-Centrum der Friedrich-Alexander-Universität Erlangen-Nürnberg, Nägelsbachstr. 25, 91052 Erlangen
and
Centre for Molecular Design, University of Portsmouth, King Henry Building, Portsmouth PO1 2DY, UK.

Molecular modeling and its application in both drug design and materials modeling is increasingly limited by its own modesty (or lack of imagination) and a failure to appreciate the capabilities of modern hard- and software. We tend to perform calculations that are not truly predictive for ever more molecules, rather than trying to get something right by investing in the physical model.

The ***hpCADD***[1] project is an attempt to rectify this trend and to initiate a step change in the way that computer-aided drug design interacts with the experimental research and development process.

At the same time, the domain of molecular modeling can now be extended into new areas that have thus far been the subject of only limited attention. Modeling organic electronic devices is one such area.

The lecture will describe new techniques and software designed to take advantage of the features of modern hardware and to make a start towards truly predictive modeling.

1. www.hpcadd.com