SEMINAR IV

MOLECULAR MODELING: PROMISES AND CHALLENGES

Md. Abu Naser

Summary

Molecular modeling is usually cheaper, easier than experiments. Modeling also offers simulations under very extreme conditions (for example in very high temperature and pressure), which is not yet physically possible. Therefore, in recent years molecular modeling gaining huge interest in scientific community. This talk has two parts: first part will cover my PhD work which shows some promises of modeling of protein surface interaction; while the second part will cover some of the challenges that have been faced in order to model a catalytic reaction in my current post doctoral research training. In both parts, background information, some results and further studies will be discussed. Possible applicability of molecular modeling in agricultural research will also be hinted. Computational details will be discussed very briefly and mathematical details will be avoided to make the presentation accessible to the audience of all levels. Areas of studies are emphasized more than the techniques used. However, limitations of the techniques will be mentioned whenever appropriate.

In the first part, I intended to discuss about protein adsorption and its usefulness or necessity to do research in this area. I used barley lipid transfer protein as a model protein and the two interfaces such as, water-vacuum and water-decane was considered to observe the conformational changes in these two interfaces. An acid called hop acid which is known as a denaturing agent of the protein also included in the modeling to enhance the unfolding of barley lipid transfer protein in the water-vacuum interface. The results of the simulations showed some promising results which will be presented to some detail in the presentation.

The second part of the talk will discuss about modeling of methanolysis reaction mechanisms using quantum mechanical technique. Detailed background information on methanolysis reaction will be given. The modeling was performed in the gas phase and the gas phase calculations have provided a very erratic result which contradicts the real experimental results and in some cases, it is proved to be difficult to observe certain mechanism of the reaction. The necessity of including solvent in the model has been felt inevitable and challenging.

Student of PhD, School of EPS-Chemistry, Henot-Watt University, Edinburgh, UK. The seminar was presented in SAU Conference Room on January 7, 2009.