

**Application of Ab-Initio Principles for  
Prediction of Chemical Reactivity**

Sanjeev Saraf, W.J. Rogers, and M.S. Mannan

Mary Kay O'Connor Process Safety Center

Chemical Engineering Department

Texas A&M University

College Station, Texas 77843-3122

**Abstract**

In order to simulate the behavior of chemical reaction or unit operations, thermodynamic, kinetic or mechanistic information is usually necessary. Such data are usually obtained from direct experimental measurements, empirical correlations, or by estimation. Data also can be obtained from molecular simulation. Prediction of reaction rates from first principles allows comparisons between theory and experiment and hence determination of reaction mechanisms on the molecular level. This paper combines developments of quantum chemistry and computer algorithms to predict reaction rate constants based on transition state theory (TST) and variational TST. The article also explores the use of commercial molecular simulation software for the initial stages of process design.