

Panatpong Hutacharoen
Acceptance Speech

First of all I'd like to thank the Anglo-Thai Society for an opportunity for me to be here today. It is my great privilege to be selected for the Educational Awards for Excellence in the area of engineering and technology. I also would like to acknowledge my supervisors: Prof. Claire Adjiman, Prof. Amparo Galindo and Prof. George Jackson whom is also here today and my sponsor Pfizer, Inc.

Before I joined in the Molecular System Engineering group at Imperial College, I worked in a medical chemistry laboratory synthesizing, charactering and purifying compounds. Of course it involves many trials and errors and decisions are pretty much made heuristically. I thought experiments could be better designed by a more systematic approach which could be obtained using theory.

Moving to Imperial, my PhD project is to develop advanced molecular engineering approaches to predict thermodynamic properties from the molecular structure. Together in the MSE group, we have developed molecular-based models based on the Statistical Associating Fluid Theory to predict complex interaction of aqueous systems which are known to be challenging. This work leads us to an accurate prediction of octanol-water partition coefficient and solubility of active pharmaceutical ingredients which are the key property in drug design. We have also developed a novel effective approach to treat intramolecular hydrogen bond, which is prevalent in medicinal chemistry but often under-recognised and seldom predicted. This is the first time a group-contribution approach is used to model such complex interactions and is considered as an exciting step towards its development. Our work has a broad range of application. One of the ultimate goals is to be used for the systematic design for the industrial products and processes.

Throughout my PhD, I have been very fortunate to work with Imperial College's and Pfizer's scientists and I very much look forward to passing this experience and knowledge to the next generation of our society.

Before this ends, I like to quote what Prof. Roald Hoffman, a Noble laureate in Chemistry (1981), said "The most important role for theory in chemistry is to provide framework in which to think, to organize knowledge". If ones say an afternoon in the library (would mean in Google Scholar nowadays) could save a month in a lab, think about how much a day in a computational lab would save us in terms of both time and resources.

Last but not least I like to thank the incomparable supports from by family and friends who are not only here joining this incredible moment but also have been standing with me through the difficult times. Thank you.