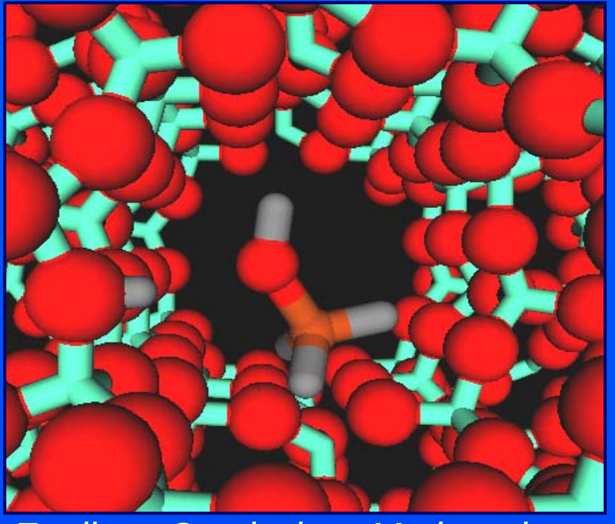
Department of Chemical &
Biomolecular Engineering

NUS
National University
of Singapore

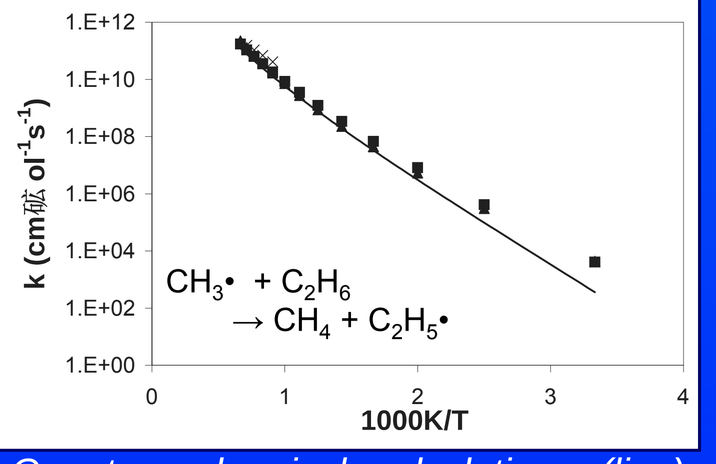
From Molecules to Processes



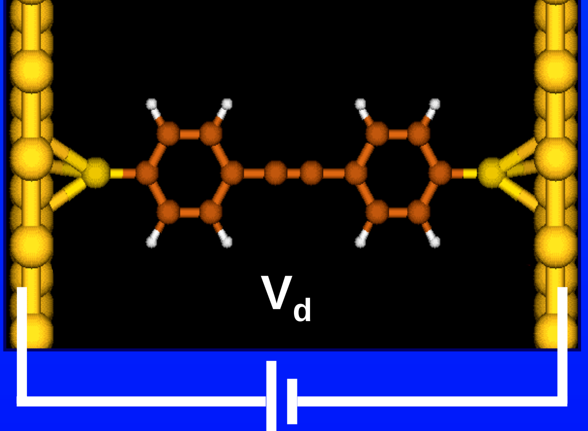
Zeolite Catalysis: Methanol to Olefins process for the production of clean fuels

How do we bridge the gap between molecular level reactions and macroscale chemical processes? Our computational chemical engineering research program seeks to link fundamental quantum mechanics to complex chemical processes at the industrial scale. Carefully selected computational procedures and state-of-the-art parallel supercomputers are used to unravel the molecular level details of complex gas-phase chemistry, catalysis, molecular electronics and biomolecular systems.

Recently we have developed methods for accurately predicting reaction rates from quantum chemistry. Thanks to the ever-increasing computational power, this new approach is rapidly becoming an important tool for the design and optimization of chemical processes.



Quantum chemical calculations (line) can predict experimental reaction rates (data points)



Molecular electronics: Simulation of nano-electronic devices

Currently we are developing new molecular modeling tools to provide a better understanding of molecular eletronics as well as biological systems, paving the way for new generations of nano-electronic devices and improved biomolecular processes.

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