Applications of DFT to chemical, materials, and biological systems: successes, failures, ideas for improvements.

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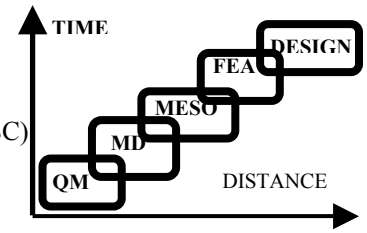
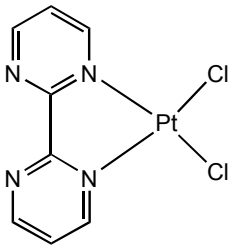


Advances in the accuracy and generality of functionals for Density Functional Theory have enabled first principles predictions of numerous important systems and processes in the Chemical, Biological, and Materials Sciences. Indeed DFT including Generalized Gradient Approximations with some exact exchange (hybrid methods) have become the method of choice for such applications. We will discuss some of these successes with applications on topics such as:

- Design of new homogeneous catalysts (CH_4 activation, polymerize polar olefins)
- Decomposition Mechanism of high energy molecules (RDX, HMX)
- Singlet oxygen oxidation of water in antibodies and the Peroxone process.
- De novo Force Fields (from QM) to describe reactions and phase transitions
- Prediction of current/voltage in nanoelectronic devices
- Electronic states of Cuprate superconductors.



Despite the successes, there are also notable difficulties involving for example

- Spin states of transition metal complexes
- Van der Waals complexes
- Electronic excited states

We will discuss some possible directions for improvements.