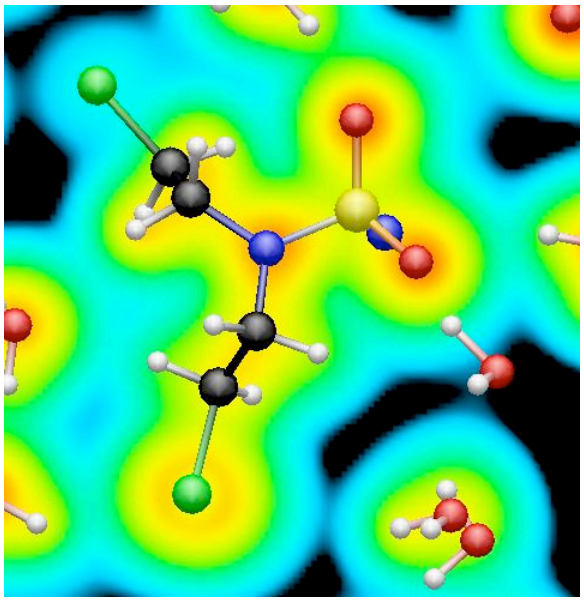
# 100+ TeraFLOP Computers Enable First Principles MD simulations of Enzyme Mechanisms

**We have been using FPMD to simulate the chemical reactions**

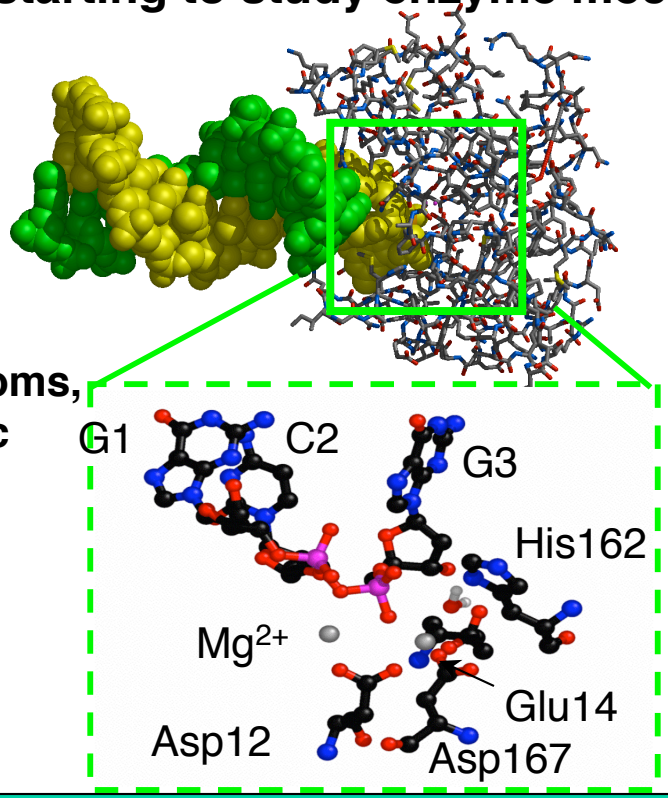


**Constrained FPMD simulations of drug with 70 water molecules (231 atoms total) ~80,000 basis functions**

**Computational requirements:**
**ASCII blue: 1ps on 36 nodes takes 5 days**
**TC2K: 1ps on 27 nodes takes 3.1 days**

M. Colvin

**We are starting to study enzyme mechanisms**




## Long-term GTL applications:

- Design of $O_2$ resistant hydrogenases
- Re-engineering substrate specificity of degradative enzymes
- Modify properties of DNA-binding regulatory enzymes