



The “3 Pillars” Approach to R&D

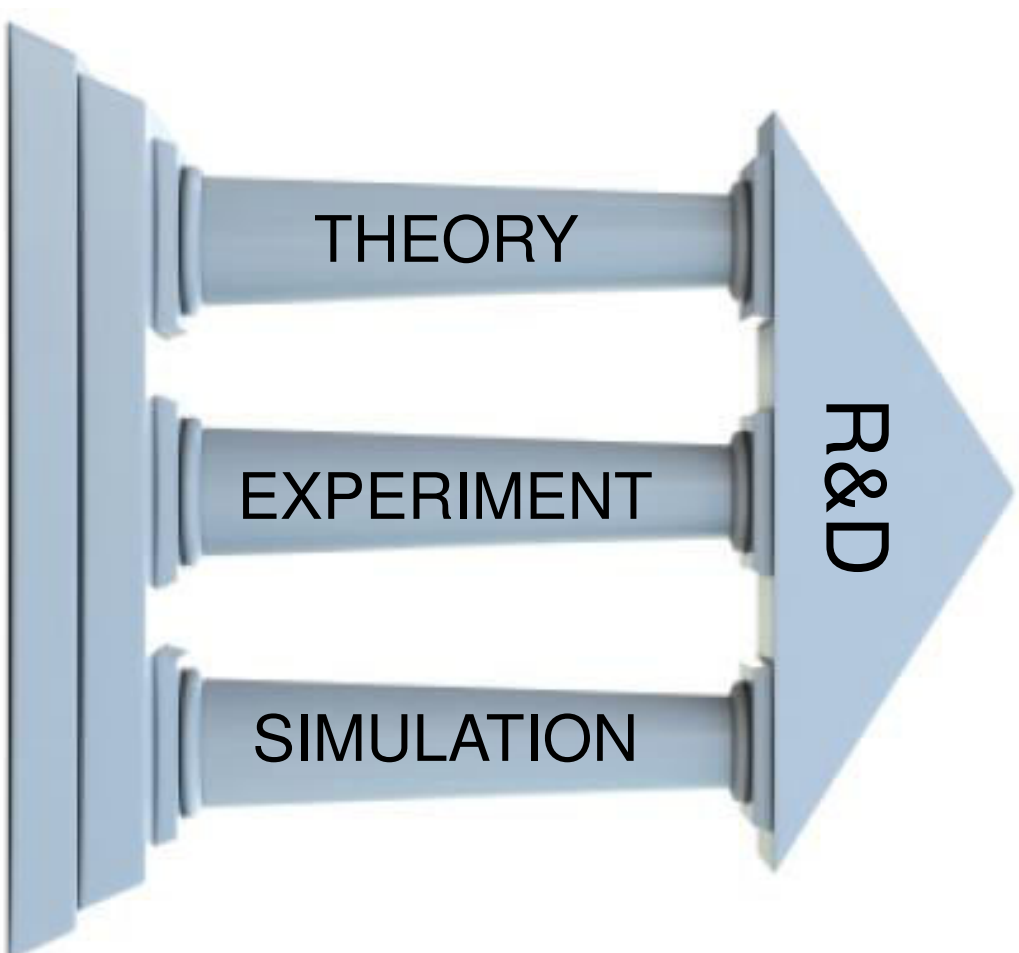
Barbara Montanari

Principal Scientist

Leader, Theoretical and Computational Physics Group

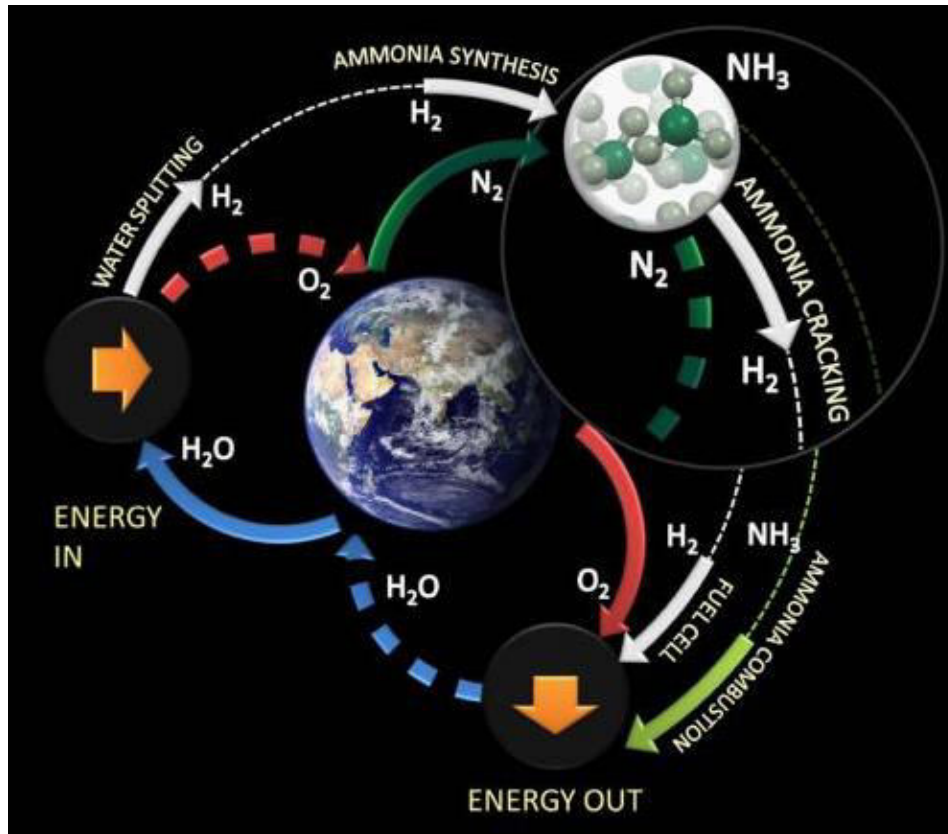
Deputy Head, Applications Division

The Three Pillars



Energy & Environment

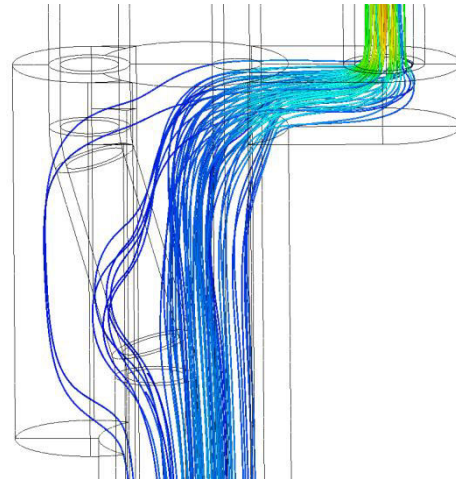
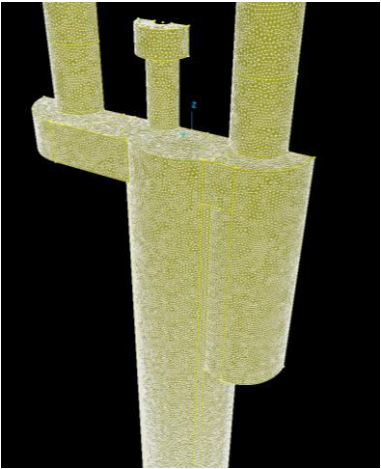
Game changer in the use of hydrogen as a "green" fuel.



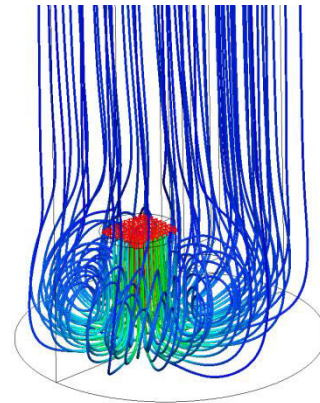
Dr Martin Jones and Prof. Bill David (ISIS)



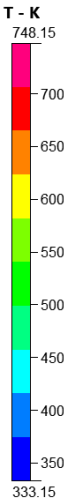
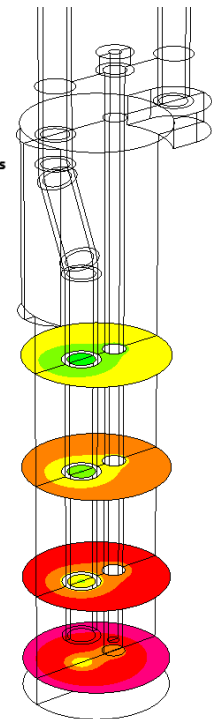
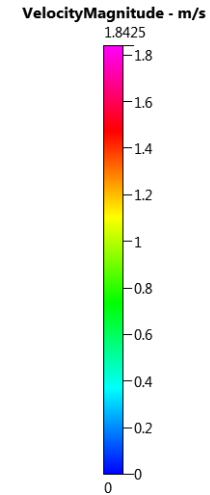
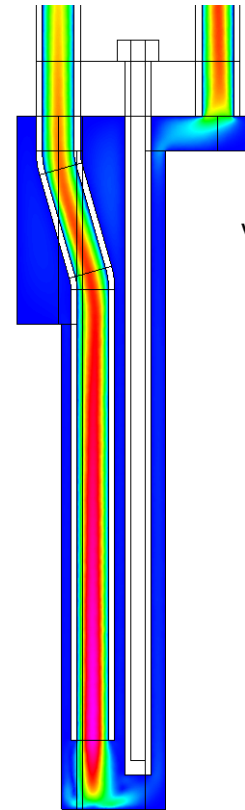
Computational Fluid Dynamics Simulations of the Reactor



Upper part of reactor



Lower part of reactor



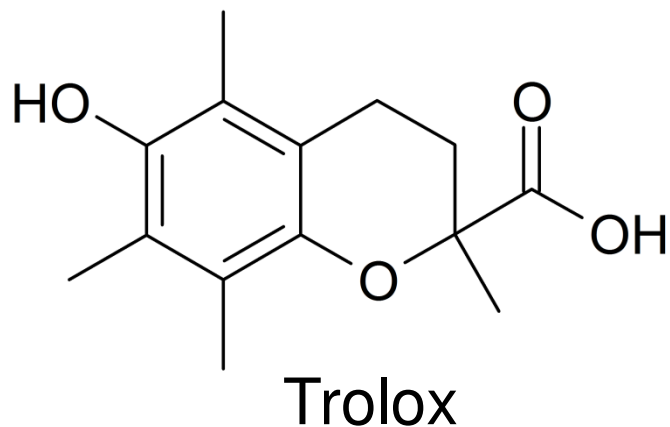
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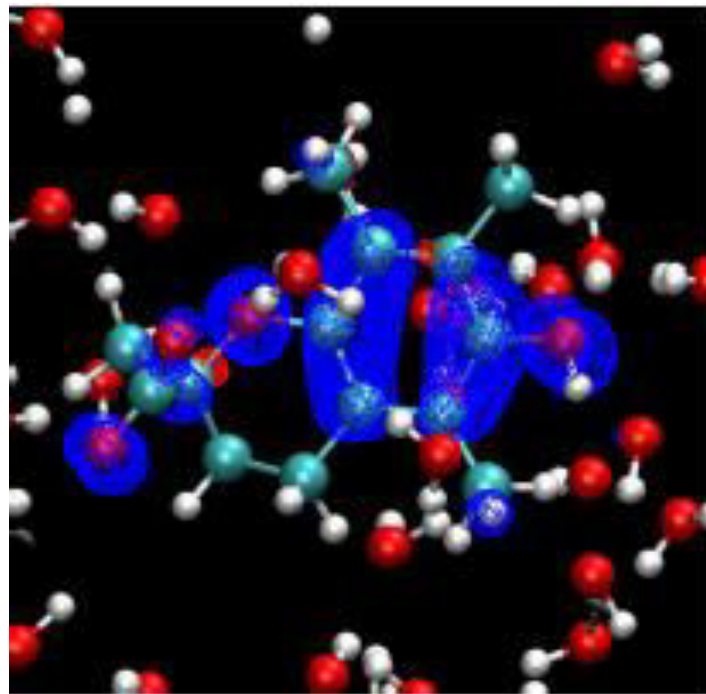
Science & Technology
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D. Emerson & R. Barber (SCD)

Healthcare: Antioxidants



- Ab initio Molecular Dynamics
- Thermodynamics
- Chemical Reactivity



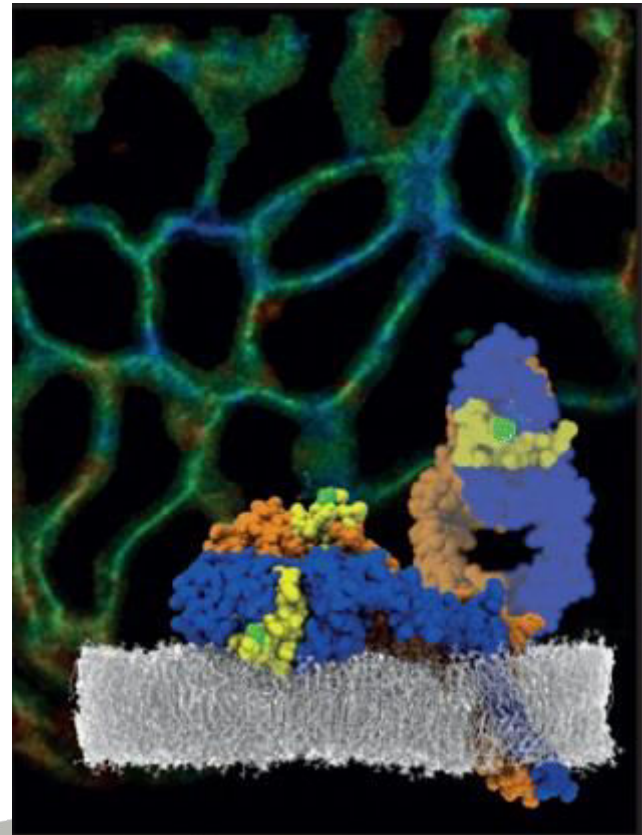
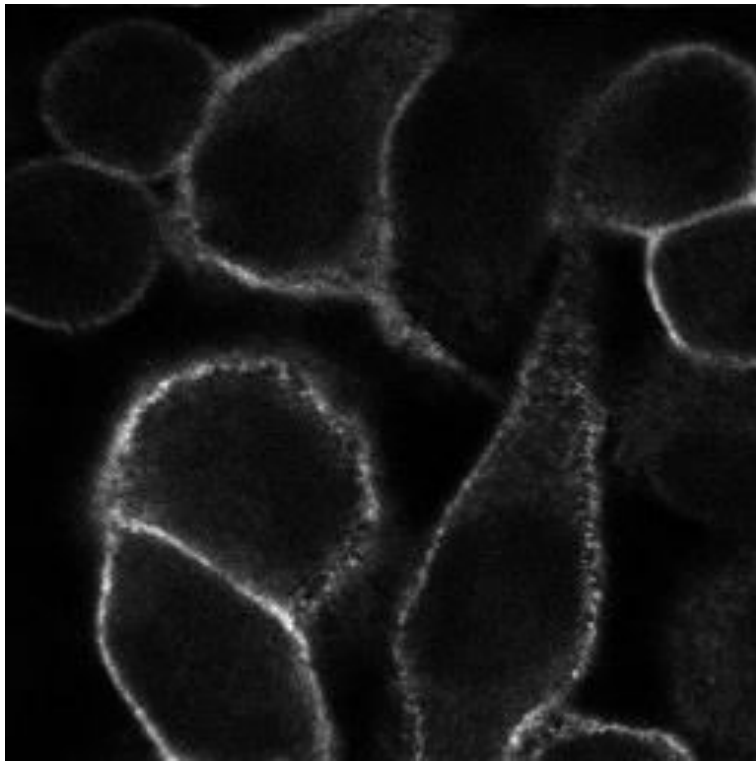
T. Parker (CLF)
L. Bernasconi and B. Montanari (SCD)



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Healthcare: Cancer Care

CLF/SCD Study of Epidermal Growth Factor Receptors



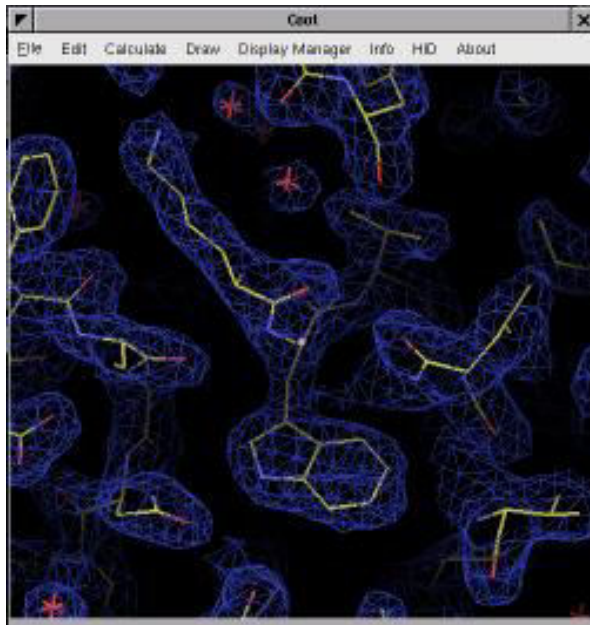
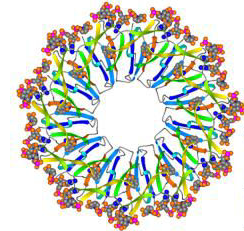
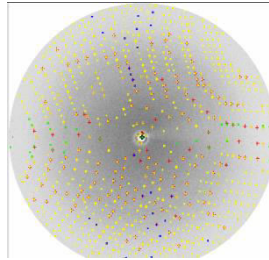
Science Signalling (2014)



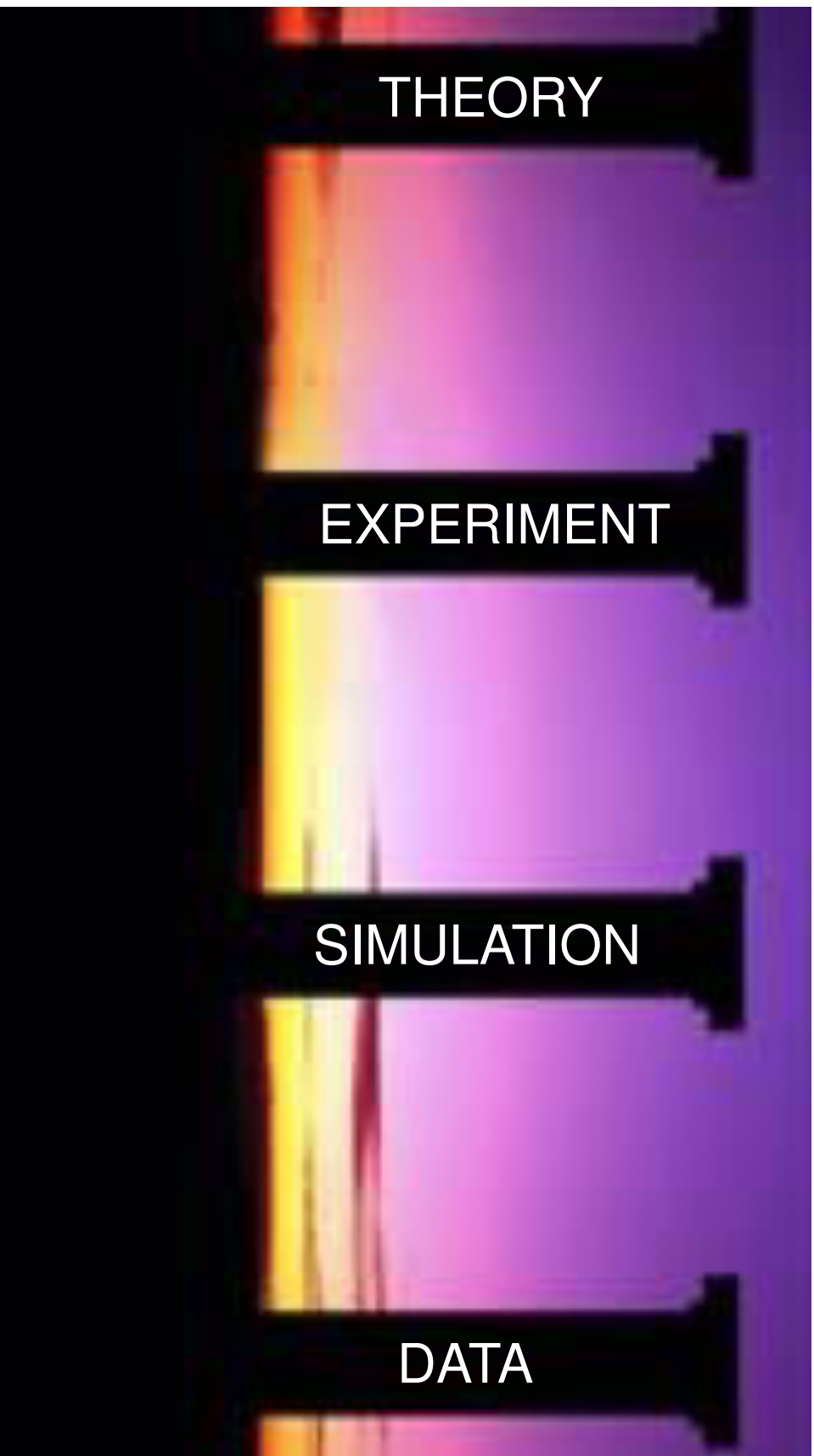
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Healthcare: Protein Structure

Data analysis for
macromolecular X-ray
crystallography

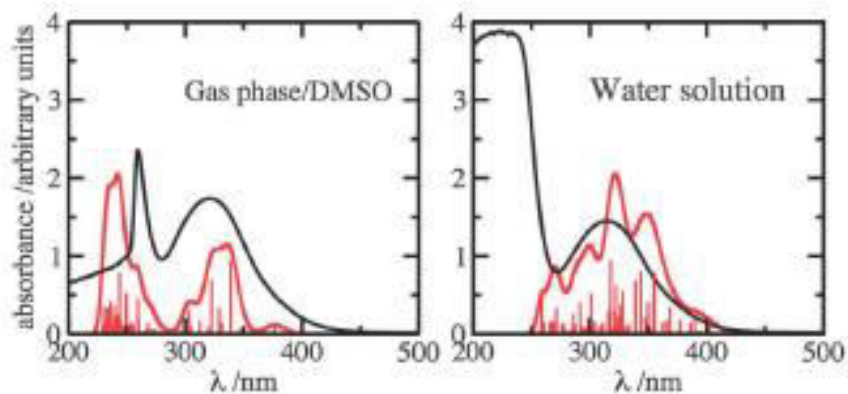
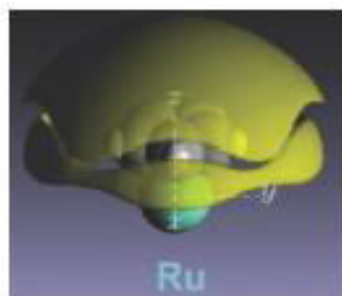
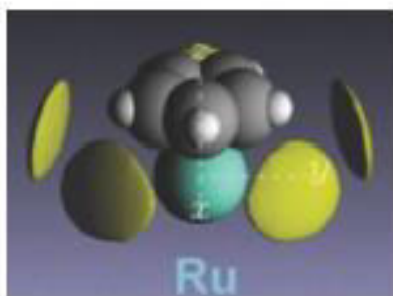


The Future: Four Pillars



Environment

Environmentally friendly homogeneous catalysis



- CRYSTAL (L. Bernasconi, SCD)
- SANDALS (S. Imberti, ISIS)