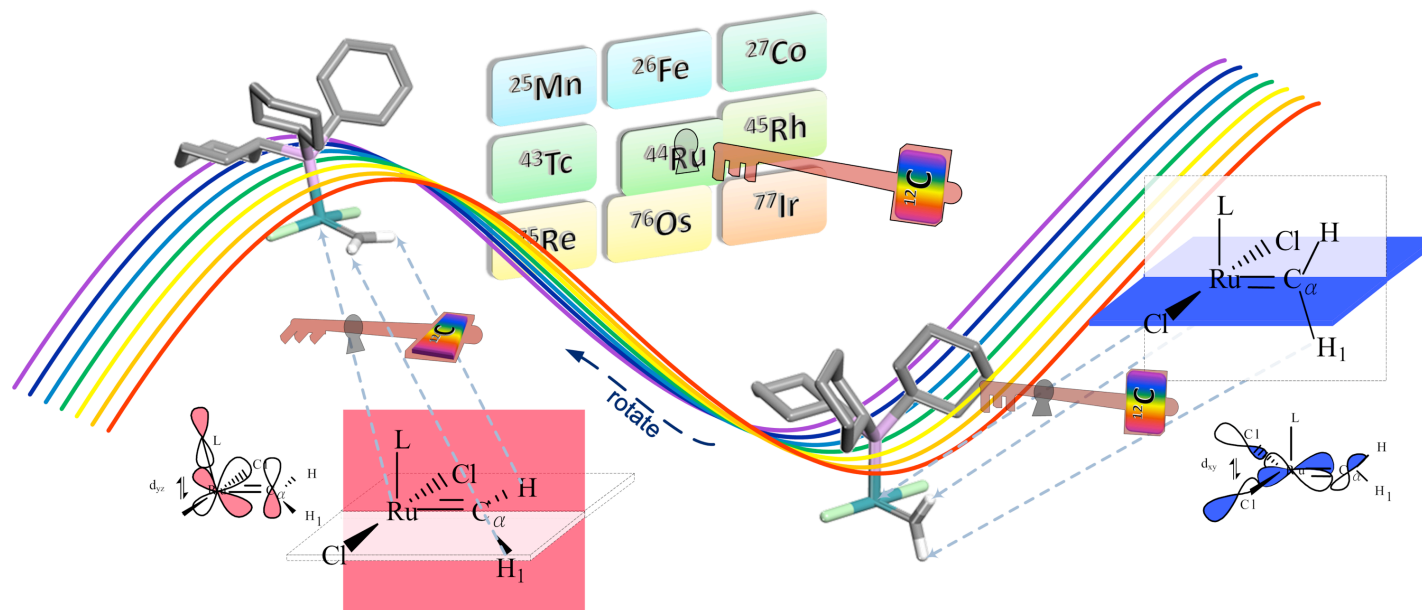


Yang, Zhao, and Truhlar
NSF research, Feb. 2011



Grubbs was awarded the Nobel Prize for developing Ru carbene catalysts for olefin metathesis, especially the second-generation catalysts.

The work with Yang and Zhao with the Minnesota density functionals has greatly increased our understanding of the mechanism:

- explained the higher activation energy for forming the second-generation catalysts.
- elucidated the unexpected role of attractive noncovalent interactions, a new concept for guiding catalyst design
- explained how ligand binding is coupled to the rotameric state of the carbene, providing a possible future route to designing stereospecific catalysts.