

Ab Initio Molecular Dynamics & Simulation Analysis Tools

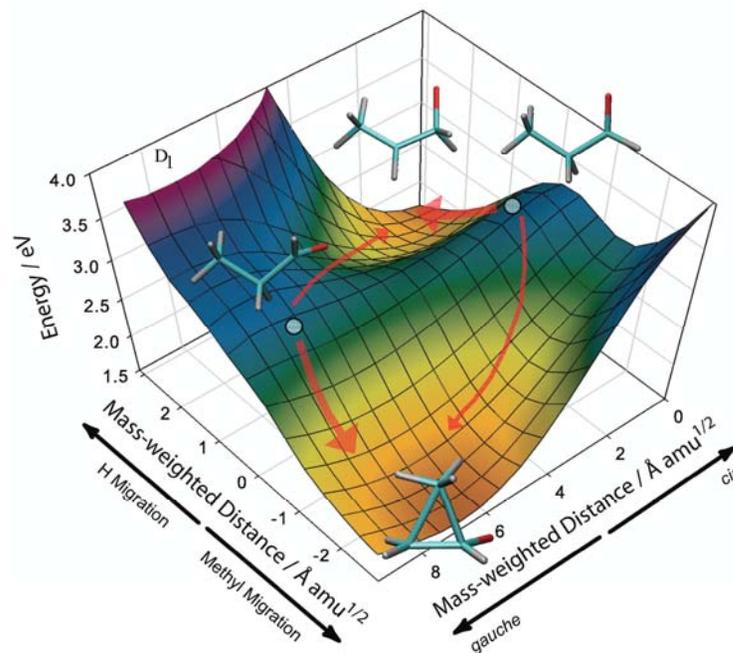
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Computer simulation can now *predict* chemical reaction dynamics, even in challenging cases. So far, this capability has been reserved for experts in the field.

Our project is accelerating widespread application of this technology by creating user-friendly tools aimed at non-experts and experimentalists. We have created the SimDB system which tracks simulations through a database accessed by a web browser and enhanced the MacMolPlt program for visualization of simulation results. These tools will make it easier to run simulations and analyze the results, leading to faster turnaround time for molecular design in applications such as materials and drug discovery.



Using the tools developed in this project, we recently explained puzzling experimental results of conformer-dependent reactivity after photoexcitation. The excited state potential energy surface favors formation of distinct products when different conformers are excited.¹ This is in spite of a very small conformational barrier in both the ground and excited states.

¹Kim, Shen, Tao, Martinez, and Suits, *Science* **315**, 1561 (2007)