

## A Priori Prediction of Radical-Radical Combination Reaction Rates

- Radical-radical combination reactions are important in combustion, atmospheric and interstellar chemistry but experimental studies of these reactions are difficult and prior theoretical treatments have been limited to small radicals.
- A new, a priori, theoretical approach has been developed that couples efficient and accurate quantum chemistry and reaction rates theories with large scale parallel computing techniques.
- The new approach has been successfully applied to both self and cross combinations of hydrogen, methyl, ethyl, iso-propyl, and tert-butyl radicals, answering a longstanding debate about temperature dependence; the rate coefficients decrease with increasing temperature.
- Work in progress is extending this approach to reactions of H atoms with resonantly stabilized hydrocarbon radicals.

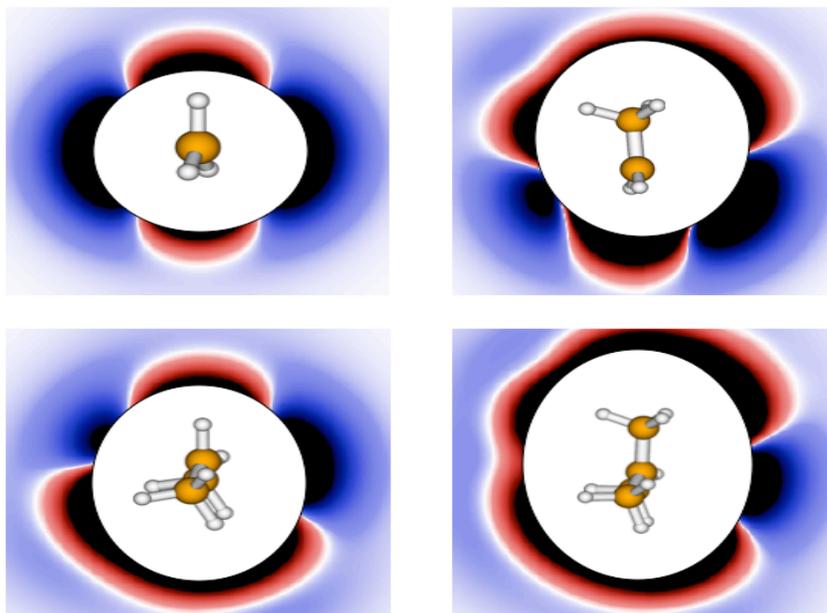


Figure: Methyl+alkyl radical CASPT2 interaction potentials. Blue regions are attractive and red are repulsive.

### References:

- L. B. Harding, Y. Georgievskii, and S. J. Klippenstein,  
*J. Phys. Chem. A* **109**, 4646 (2005).  
S. J. Klippenstein, Y. Georgievskii, and L. B. Harding,  
*Phys. Chem. Chem. Phys.* **8**, 1127 (2008).