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.

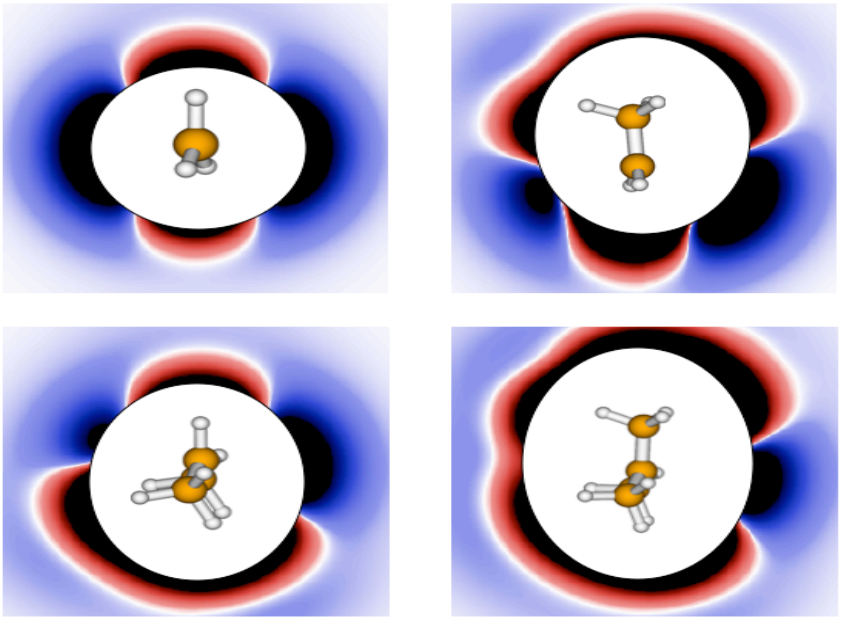

Figure: Methyl+alkyl radical CASPT2 interaction potentials. Blue regions are attractive and red are repulsive.

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