Quantum Dynamics Revealed

***Objective*: Study detailed quantum dynamics of elementary chemical reactions in the gas phase and on surfaces.**

***Implications*: These elementary reactions are often at the heart of important processes in combustion and catalysis.**

- ***Accomplishments:*** **Detailed calculations of O+OH➔H+O_2, which is the reverse of the most important combustion reaction and is also important for ozone destruction, shed light on long-standing questions about the statistical nature of the reaction dynamics.**
- **Results will serve as a benchmark for more approximate treatments.**

NERSC: **Codes using OpenMP parallelism for calculating both total and differential cross sections were developed on Franklin and Hopper; NERSC NISE award, 2010**

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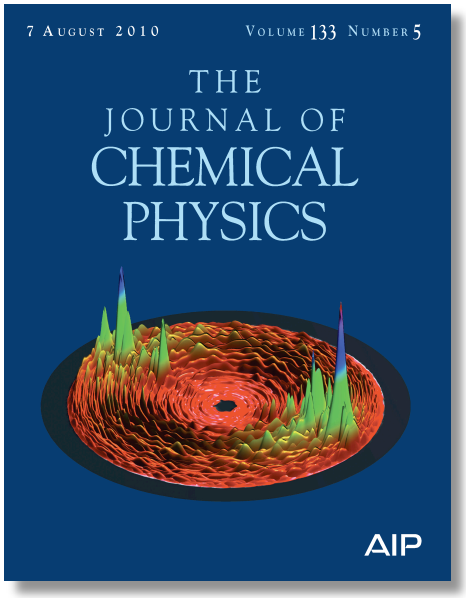

The cover image shows a polar-coordinates plot of differential cross sections for the O+OH reaction at 150meV of collision energy. The article was one of the top-20 most downloaded papers from this issue.

State-to-state quantum dynamics of the $O(^3P)+OH(^2\Pi)\rightarrow H(^2S)+O_2(^3\Sigma_g^-)$ reaction

Journal of Chemical Physics 133, 054302, August 7, 2010 (cover story)

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