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Accurately Predicting Complex Reaction Kinetics from First Principles

WILLIAM GREEN, Massachusetts Institute of Technology

Many important systems contain a multitude of reactive chemical species, some of which react on a timescale faster than collisional thermalization, i.e. they never achieve a Boltzmann energy distribution. Usually it is impossible to fully elucidate the processes by experiments alone. Here we report recent progress toward predicting the time-evolving composition of these systems a priori: how unexpected reactions can be discovered on the computer, how reaction rates are computed from first principles, and how the many individual reactions are efficiently combined into a predictive simulation for the whole system. Some experimental tests of the a priori predictions are also presented.