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Transferable kinetic Monte Carlo models of condensed phase high temperature chemistry learned from molecular dynamics data.[1] QIAN YANG, University of Connecticut, ENZE CHEN, VINCENT DUFOUR-DECIEUX, Stanford University, CARLOS SING-LONG, Pontificia Universidad Catolica de Chile, RODRIGO FREITAS, EVAN REED, Stanford University — Complex chemical processes such as the decomposition of energetic materials are typically modeled at the atomistic level using large-scale molecular dynamics simulations (MD), generating a wealth of data. We propose that these rich and expensive datasets can be reused systematically to study related systems, reducing the number of new MD simulations required. We develop a statistical learning framework for extracting information about the fundamental underlying reaction pathways observed from MD data, using it to build kinetic Monte Carlo models (KMC) of the corresponding chemical reaction network. We show how and why our KMC models can predict the dynamics of entirely different chemical trajectories. We demonstrate our framework throughout on different systems of high temperature, high pressure liquid hydrocarbons. One can easily imagine a future in which MD simulations used for research are routinely archived and analyzed in order to add to and modify an existing repository of elementary chemical reactions and reaction rates. This repository would form a "chemical genome" that can then be used to quickly simulate all kinds of new chemical systems.

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