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A Novel Approach to Kinetics on Complex Potential Energy Surface JUN LU, R. STEPHEN BERRY, Department of Chemistry and The James Franck Institute, The University of Chicago — Understanding the kinetics and dynamics of the underlying potential energy surface (PES) is essential to many scientific problems, e.g. the dynamics of the molecular clusters and polymers, the folding of proteins, the complicated phenomenology of glasses, and even the optimal design of nanoparticle materials. However, the complexity and the huge number of dimensions of the PES of typical systems of interest forces us to statistically simplify it in order to understand and even manipulate the underlying kinetics. These challenges are addressed by using a novel approach of constructing PES-like networks of stationary points. If constructed with proper regularity, the kinetics of the artificial PES is easy to predict and understand; thus by tuning the stationary points in these PES networks, we have a useful channel to study the complexity of kinetics on an irregular PES. The Master Equation is used to study the kinetics on a PES and the strategies of statistical sampling for a multi-dimensional surface. It is the largest eigenvalues and their corresponding eigenvectors that provide the most important kinetic information. Furthermore, one can measure the robustness of the sampling strategies by comparing the eigenvalue and eigenvector spectra of full and sample PESs.

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