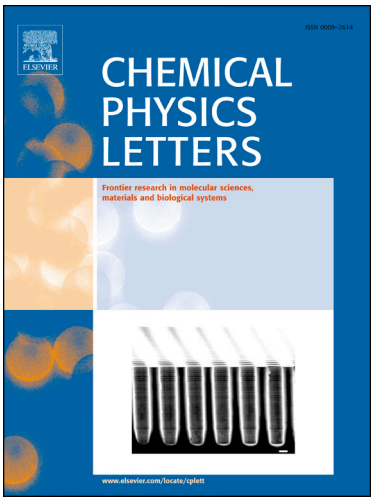

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Mean Field Treatment of Heterogeneous Steady State Kinetics

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Abstract

We propose a method to quickly compute steady state populations of species undergoing a set of chemical reactions whose rate constants are heterogeneous. Using an average environment in place of an explicit nearest neighbor configuration, we obtain a set of equations describing a single fluctuating active site in the presence of an averaged bath. We apply this Mean Field Steady State (MFSS) method to a model of H_2 production on a disordered surface for which the activation energy for the reaction varies from site to site. The MFSS populations quantitatively reproduce the KMC results across the range of rate parameters considered.

Introduction

Beneath the ensemble average common to macroscopic observations, heterogeneity plays an astonishing role in chemical kinetics. From light harvesting [1] to chemical catalysis [2] to signaling [3] to enzyme function [4] there is a common theme: chemical function is not determined by the typical or average member of the ensemble. Rather, the rate of a given process can be strongly influenced by outliers.

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