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An Efficient Kernel Polynomial Method for Calculating Transition Rates in Large-Scale Materials[1] CHEN HUANG, ARTHUR VOTER, DANNY PEREZ, Los Alamos National Laboratory — We present an efficient method for calculating transition rates in large-scale materials using harmonic transition state theory. In this method, we first reformulate the prefactor of the transition rates in terms of the density of states (DOS) of Hessian matrices. The DOS are then efficiently calculated with the kernel polynomial method. The scaling of our method is discussed in detail. We demonstrate our approach by calculating the prefactors for vacancy hopping and Frenkel pair formation in silver. Very good agreement between the KPM approach and exact diagonalization is observed.

[1]DOE/BES and DOE/ASCR

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