

Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Biased Monte Carlo technique to accelerate Molecular Dynamics simulations of rare events PRATYUSH TIWARY, AXEL VAN DE WALLE, Department of Applied Physics and Materials Science, Caltech — We propose a hybrid Monte Carlo (MC) -Molecular Dynamics (MD) technique to study temporally rare event dynamics. By using biased MC sampling (Metropolis-Hastings), we avoid actually visiting low energy states in the MD and instead carry out a quick estimate of the mean escape time to be added to the computer clock. The method does not assume anything about the nature of the transition surfaces separating basins in the energy surface. We then apply the method to the case of dislocation kink movement in BCC metals at low temperatures.

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Date submitted: 23 Nov 2010

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