

Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Optimization of constant pH replica exchange molecular dynamics method DANIAL SABRI DASHTI, Beckman Institute, University of Illinois, Urbana, IL, 61801, USA, ADRIAN ROITBERG, Department of Chemistry and Quantum Theory Project, University of Florida, Gainesville, FL, 32611, USA — Improvement in sampling of configuration space enhances sampling in protonation space. Recently a constant pH replica exchange (PHREM) method has been developed by Itoh et al to improve the coupling between conformational and protonation sampling. We present a technique for estimating the exchange acceptance ratio (EAR) between two arbitrary replicas (i.e., with distinct pHs) in PHREM. Moreover, we designed a scoring function to optimize the position of each replica on pH ladder. Maximizing the scoring function results in equal EAR between all neighbor pairs, which increases the efficiency of PHREM. We have tested our method on erabutoxin and hen egg white lysozyme (HEWL). We found that the estimations of pKa values in the optimized set of replicas converge faster respect to equally spaced set.

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Date submitted: 15 Nov 2013

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