Abstract Submitted
for the SHOCK13 Meeting of
The American Physical Society

Parameterization of classical force fields in the context of high pressure calculations BRANDON YANCIW, JEFFERY PERKINS, BRANDON WIEBE, University of the Fraser Valley, JACOB SPOONER, Simon Fraser University, NOHAM WEINBERG, University of the Fraser Valley, Simon Fraser University
— Activation volumes and volume profiles of chemical reactions are concepts widely used in high pressure reaction kinetics. We have recently shown that these quantities can be calculated using molecular dynamics (MD) simulations with accuracy comparable to that of the experiment. The major challenge in performing such calculations comes from the fact that standard MD force fields are parameterized for stable species and, therefore, are not directly usable for transient points along the reaction coordinate. We propose a consistent scheme of parameterization for such species based on fitting force field potentials to quantum mechanical deformation energies, and show that MD simulations with these parameters produce molar volumes of quality comparable to that of OPLS and the experiment.

Brandon Yanciw
University of the Fraser Valley

Date submitted: 20 Feb 2013 Electronic form version 1.4