Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Order parameter aided phase space exploration under extreme conditions[1] AMIT SAMANTA, SEBASTIAN HAMEL, ERIC SCHWEGLER, Lawrence Livermore National Laboratory — Efficient exploration of configuration space and identification of metastable structures in condensed phase systems are challenging from both computational as well as algorithmic perspectives. In this talk I will illustrate how we can extend the recently proposed order-parameter aided temperature accelerated sampling schemes to efficiently and systematically explore free energy surfaces, and search for metastable states and reaction pathways within the framework of density functional theory based molecular dynamics. I will illustrate how this sampling scheme can be used to explore the relevant parts of configuration space in prototypical materials, like SiO2 and identify the different metastable structures, transition pathways and phase boundaries.

[1]This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

Amit Samanta
Lawrence Livermore National Laboratory

Date submitted: 05 Nov 2015 Electronic form version 1.4