4th International Symposium on
Energy Challenges & Mechanics
- working on small scales

11-13 August 2015
Aberdeen, Scotland, UK

Massively Parallel Reactive and Quantum Molecular Dynamics Simulations

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Accepted for publication on the 7th of February 2015

In this talk I will discuss two simulations:

Cavitation bubbles readily occur in fluids subjected to rapid changes in pressure. We use billion-atom reactive molecular dynamics simulations on a 163,840-processor BlueGene/P supercomputer to investigate chemical and mechanical damages caused by shock-induced collapse of nanobubbles in water near silica surface. Collapse of an empty nanobubble generates high-speed nanojet, resulting in the formation of a pit on the surface. The gas-filled bubbles undergo partial collapse and consequently the damage on the silica surface is mitigated.

Quantum molecular dynamics (QMD) simulations are performed on 786,432-processor Blue Gene/Q to study on-demand production of hydrogen gas from water using Al nanoclusters. QMD simulations reveal rapid hydrogen production from water by an Al nanocluster. We find a low activation-barrier mechanism, in which a pair of Lewis acid and base sites on the Al_n surface preferentially catalyzes hydrogen production. I will also discuss on-demand production of hydrogen gas from water using and LiAl alloy particles.

Keywords: Reactive Molecular Dynamics Simulations; Nanobubble Collapse; Chemo-mechanics; Aluminum nanoparticles in water; Hydrogen production