Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

SUPPLEMENTARY INFORMATION

ReaxFF Based Molecular Dynamics Simulations of Ignition Front Propagation in Hydrocarbon/Oxygen Mixtures under High Temperature and Pressure Conditions

Chowdhury Ashraf, Abhishek Jain, Yuan Xuan and Adri C.T. van Duin

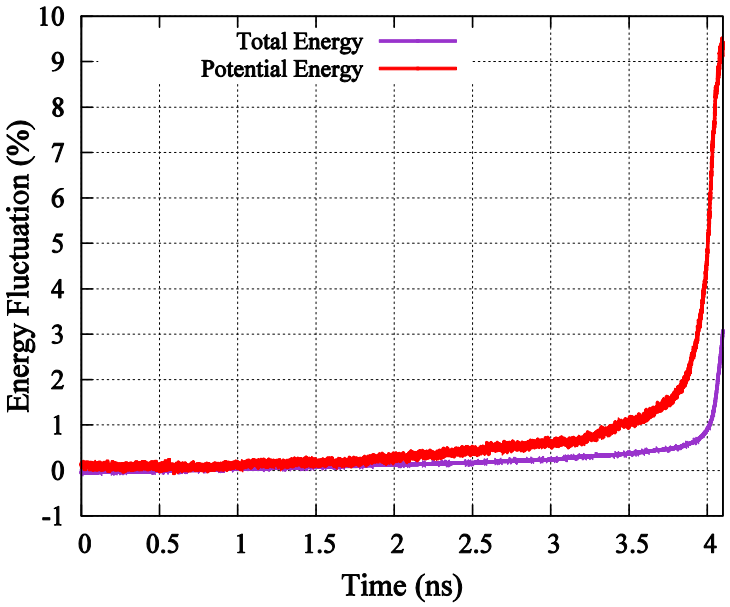

Figure S1: Fluctuation of total energy and potential energy with time for toluene simulation. Fluctuation of total energy is significant only after 4ns, before that the fluctuation is small compared to potential energy fluctuation. Our ignition speed calculation is based on first 4ns simulation only.