

Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Structure and Dynamics of Water Confined in Graphitic Nanostructures¹ YUZI HE, RAJIV KALIA, AIICHIRO NAKANO, PRIYA VASHISHTA, Collaboratory of Advanced Computing and Simulations Department of Physics and Astronomy, University of Southern California — We study the structure and dynamics of water confined in nanocarbon ribbons and graphitic nanostructures using reactive molecular dynamics (RMD) simulations based on reactive force fields. The nanocarbon ribbons and graphitic nanostructures are generated in an RMD simulation of oxidation of a silicon carbide nanoparticle. We find that Si oxidizes rapidly and nanocarbon ribbons and graphitic nanostructures are a byproduct of Si oxidation. We embed water molecules in graphitic nanopores and study structural and dynamical properties of nanoconfined water as a function of temperature and pressure. RMD simulation results indicate the presence of high density water (HDW) and low density water (LDW). Results for the effect of high pressure and supercooling on the dynamics of water will be reported.

¹This work was supported as part of the Computational Materials Sciences Program funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.

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Date submitted: 09 Nov 2016

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