Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Computational studies of carbon-onions for electrochemical capacitor applications P. GANESH, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, P.R.C. KENT, Center for Nanophase Materials Sciences and Computer Science and Mathematics Division, V. MOCHALIN, Department of Materials Science and Engineering, Drexel University, LUKAS VLCEK, Chemical Sciences Division, Oak Ridge National Laboratory Oak Ridge, ADRI VAN DUIN, Department of Mechanical and Chemical Engineering, Penn State University — Supercapacitors bridge the gap between conventional batteries and electrolytic capacitors. Recently, onion-like carbon structures have [1] shown to have capacitances four orders of magnitude higher and energies an order of magnitude higher than conventional capacitors, making them the fastest growing competitors for energy storage. We study the formation of carbon-onions from nanodiamonds using reactive force-fields [2]. Our study suggests that the temperature and mechanical stability as well as the final-equilibrium structure are strongly dependent on the inclusion of long-range forces. We are currently developing reactive-force fields to allow mesoscopic modeling of reactions of carbon nanostructures with aqueous electrolytes. Progress along these lines will also be presented. This material is based upon work supported as part of the Fluid Interface Reactions, Structures and Transport (FIRST) Center, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences.

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[2] Adri C. T. van Duin et.al, J. Phys. Chem. A 105, 9396 (2001)

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Date submitted: 23 Nov 2011 Electronic form version 1.4