Condensed Matter Physics

DETERMINISTIC COMPUTER SIMULATIONS OF HYDROGEN STORAGE IN CARBON NANOSTRUCTURES, *M. Kaspar,[1] M.W. Roth[1*], T.E. Kidd[1], L. Strauss[2] and M.J. Connolly[3], [1]Department of Physics, University of Northern Iowa, Cedar Falls, IA 50614, [2]Department of Chemistry and Biochemistry, University of Northern Iowa, Cedar Falls, IA 50614, [3]University of Missouri, Department of Physics and Astronomy, Columbia, MO 65211, corresponding author email: rothm@uni.edu*

Hydrogen storage is of great importance for the world of tomorrow; as an essentially pollutant free energy source it shows great promise for reducing the world's pollution. A current challenge, however is its having low energy density by volume when compared to hydrocarbons. With the use of Molecular Dynamic Simulations we are capable of studying hydrogen storage in graphite and other materials at extreme temperatures and pressures in a safe matter such as graphene and other carbon nanostructures. We present the results of massively parallel MD simulations of hydrogen in graphene layers where the layer spacing is systematically varied.

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