CAR-PARRINELLO MOLECULAR DYNAMICS SIMULATIONS OF BORON-NITROGEN HYDRIDES

JUN LI, S.M. KATHMANN, G.K. SCHENTER, J.C. LINEHAN, S.T. AUTREY, and M. GUTOWSKI, *W.R. Wiley Environmental Molecular Sciences Laboratory and Fundamental Science Directorate, Pacific Northwest National Laboratory, Richland, WA 99352*.

Hydrogen storage materials have aroused great interest in both fundamental and applied research in the past several years. Boron-nitrogen hydrides (BNH_x) such as ammonia borane, BH_3NH_3, are one of the most promising hydrogen storage materials because of their high gravimetric and volumetric densities of hydrogen. In this talk, we will present theoretical results on some $H(BH_2NH_2)_nH$ (n = 1-6) oligomers, which might result from dehydrogenation of BH_3NH_3 and BH_4NH_4 materials. Car-Parrinello molecular dynamics simulations and geometry optimizations have been performed to elucidate the geometries, stabilities, reactivities, and electronic structures of these oligomers and to compare with analogous hydrocarbons. Support for this work was provided through the DOE Center of Excellence for Chemical Hydrogen Storage of the Hydrogen Program at the US Department of Energy.