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A Reactive Bond Order Potential for NxHy Species: Molecular Dynamics Simulations of Hydrazine Decomposition YANHONG HU, North Carolina State University, EDWARD BYRD, BETSY RICE, US Army Research Laboratory, DONALD BRENNER, North Carolina State University, BRENNER COLLABORATION — A reactive empirical bond order potential for N_xH_y species has been developed that describes bonding properties over a wide range of molecular and solid-state structures. The function includes non-bonded interactions, and allows bond breaking and forming with appropriate changes in atomic hybridization in a computationally efficient manner, features that facilitate large-scale atomic simulations of condensed-phase reactive chemistry. Initial simulations of the chemical decomposition of hydrazine under extreme conditions will be presented and compared with available experimental results and *ab initio* calculations. Because many of the properties of hydrazine are reasonably well known from experiment, the results of our simulations will help validate the potential, as well as lend important new insights into the reactive dynamics of these systems. This work is supported by a DOD MURI grant managed by the Army Research Office.

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