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THE HIGH ENERGY DENSITY MATERIALS: A NEW CHALLENGE FOR THE FUTURE

Abstract

By definition HEDM must possess high energy density J (e.g., in Joule/kg). This quantity depends on the potential energy associated to the binding force, where binding is a general concept not necessarily connected to atoms or molecules. Because the fundamental forces known are only three, the ROM of J associated to each force can be readily evaluated and will be discussed. For chemical bonds ultimately J depends on the electronic configuration, and that can be evaluated using quantum mechanics calculations as embodied in specialized codes. Even without such analysis, a broad range of species is known to exist that possesses high J because of their ionic state or electronic excitation. These will be presented and their potential J evaluated for application to rocket propulsion. Some new species under examination for airbreathing propulsion will also be discussed. As for the J associated to the nuclear force, the strongest known, the energy density of fission, fusion and nuclear isomers will be presented and compared to that of chemical species. For solid propellants, the current objective of the synthesis studies of new energetic molecules is to increase the enthalpy of formation and density. This trend sees its outcome with the metastable molecules. They store energy as they consist of atoms that are linked by weak bonds and break down into molecules that have much stronger bonds between atoms. The nitrogen-based compounds are good candidates because of the high energy in the nitrogen triple bond and weak energies of the double and mostly the single bond. Their study requires a particular process. The first step consists in imagining structures of nitrogen molecules and by calculating the energy of activation corresponding to their decomposition. The value of this energy must be sufficiently high so that the product is potentially usable. The enthalpy of formation and the density of the selected structures are calculated. They are far superior to those of the new molecules currently used in formulation studies of high-energy propellants. So, this kind of molecules offers an opportunity to increase dramatically the performances. Significant efforts are devoted to synthesis. This concept carries likely a long term breakthrough.