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The Quest for Greater Chemical Energy Storage II: On the Relationship between Bond Length and Bond Energy MICHAEL LINDSAY, Energetic Materials Branch, Air Force Research Laboratory, ROBERT BUSZEK, JERRY BOATZ, Propellants Branch, Air Force Research Laboratory, MARIO FAJARDO, Energetic Materials Branch, Air Force Research Laboratory — This is the second in a series of papers aimed at exploring the fundamental limitations to chemical energy storage. In the previous work, we summarized the lessons learned in various high energy density materials (HEDM) programs, the different degrees of freedom in which to store energy in materials, and the fundamental limitations and orders of magnitude of the energies involved.[1] That discussion focused almost exclusively on the topic of molar energy density (J/mol) from the perspective of the energy of oxidation of the elements and Fritz Zwicky's "free atom limit."[2] In this talk, we extend the analysis by considering a different, though equally important, aspect of the energy density calculation: the volumetric density of the energetic material. Specifically, we examine how the distances between individual atoms (i.e. intra- and inter-molecular bond lengths) are coupled to (in fact, approximately inversely proportional to) the energy stored in the bonds of the molecule. This relationship further limits the chemical energy that theoretically can be stored in a material below that predicted by the "free atom limit." This talk will give specific examples of the trends with different bonding motifs and the implications to the fundamental limitations of chemical energy storage.

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