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## ACCEPTED MANUSCRIPT

Science-based framework for ensuring safe use of hydrogen as an energy carrier and an emission-free transportation fuel

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#### **Highlights**

- Measured dust cloud explosion parameters of candidate hydrides and activated carbon.
- Identified fire / explosion risks of candidate hydrides during postulated accidents.
- Determined explosion severity, ignition sensitivity, K<sub>ST</sub> index of selected hydrides.
- Identified two novel risk mitigation strategies for selected hydrides.

<sup>1</sup> Dr. Y. F. Khalil is the current Operating Agent (OA) for the International Energy Agency (IEA), Hydrogen Safety Task. He is also the Editor-in-chief of the IEA Hydrogen Safety Journal and a member of the Hydrogen Technologies Executive Committee of the U.S. National Fire Protection Association (NFPA). DR. Khalil was the Principal Investigator (PI) for U.S. Department of Energy (DOE) Contract no. DE-FG36-07GO17032 on 'Quantifying and addressing the DOE material reactivity requirements with analysis and testing of hydrogen storage materials and systems.'

#### Abstract

The objective of this research is to examine the safety-related characteristics of candidate hydrogen storage materials being considered for use in light-duty fuel-cell vehicles (LD-FCV) under the U.S. Department of Energy (DOE) Hydrogen Program. This research aims to provide useful meaning to the general DOE safety target by establishing a link between the safety-related characteristics of candidate storage materials and satisfaction of DOE safety target. Accordingly, a science-based framework has been developed and consists of standardized materials tests (based on internationally accepted ASTM and United Nations testing protocols), novel risk mitigation strategies, and subscale system demonstration. The examined storage materials include NaAlH4, AlH3, 2LiBH4+MgH2, 3Mg(NH<sub>2</sub>)<sub>2</sub>.8LiH, NH3BH3, and activated carbon (Maxsorb AX-21). The scope of safety tests covers conditions that the storage material may encounter during postulated accident scenarios such as dust cloud explosion, materials reactivity in air and other fluids, hot-surface contact, mechanical impact, and fast depressurization. The generated insights can be useful for assigning realistic probability values needed for quantifying risk scenarios, characterizing material's hazard class, and supporting current and new hydrogen safety codes and standards. For

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