

PHYSICAL CHEMISTRY 2021

4th International Meeting
on

***Materials Science for
Energy Related Applications***

BOOK OF ABSTRACTS

September 22-23, 2021

University of Belgrade - Faculty of Physical Chemistry, Belgrade

UNIVERSITY OF BELGRADE
FACULTY OF PHYSICAL CHEMISTRY
Belgrade, Serbia

THE SOCIETY OF
PHYSICAL CHEMISTS OF SERBIA
Belgrade, Serbia



4th International Meeting
on
Materials Science for Energy Related Applications

held on September 22-23, 2021 at the
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Belgrade, Serbia
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*15th International Conference on Fundamental
and Applied Aspects of Physical Chemistry*

Organized by

**UNIVERSITY OF BELGRADE
FACULTY OF PHYSICAL CHEMISTRY
Belgrade, Serbia**

in co-operation with
THE SOCIETY OF PHYSICAL CHEMISTS OF SERBIA



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**MATERIALS SCIENCE FOR
ENERGY RELATED APPLICATIONS**

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BELGRADE, SERBIA 2021

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INTERACTION OF LIGHT ALKALI METALS WITH AMMONIA BORANE: A THEORETICAL STUDY

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Ammonia borane – AB (formula: $\text{NH}_3\text{-BH}_3$) has been known for its extraordinary gravimetric hydrogen capacity (nearly 20 wt.%) and is therefore considered as promising hydrogen storage material. However, there are several drawbacks to overcome, namely dehydrogenation kinetics is rather poor, and three-step desorption releases contaminated hydrogen with each subsequent step requiring significantly higher temperature. In addition, there are detrimental by-products (e.g., borasine, diborane) that also limit its practical application. Eliminating at least borasine release is possible through the reaction of alkali metal ($\text{M}=\text{Li}, \text{Na}$) with AB and producing monometallic amidoborane salts MAB.

In this paper, electronic structure calculations and the analysis of charge density topology of pure AB, lithium, and sodium amidoboranes were performed in order to investigate cohesion and bonding nature. The influence of the specific alkali metal substitution will be assessed using calculated IR and Raman spectra and analysis of vibrational bands in comparison to pure AB.

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