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INSTITUTE of TECHNICAL SCIENCES of SASA  
VINČA INSTITUTE of NUCLEAR SCIENCES, UNIVERSITY of BELGRADE  
HYDROGEN STORAGE INITIATIVE SERBIA**

**PROGRAM AND THE BOOK OF ABSTRACTS**

**JOINT EVENT OF THE 11<sup>TH</sup> YOUNG RESEARCHERS' CONFERENCE: MATERIALS  
SCIENCE AND ENGINEERING**

**AND**

**THE 1<sup>ST</sup> EUROPEAN EARLY STAGE RESEARCHERS' CONFERENCE ON HYDROGEN  
STORAGE**

**Edited by:**

**Jasmina Grbović Novaković**

**Nenad Ignjatović**

*Joint event of the 11<sup>th</sup> Young Researchers' Conference: Materials Science and Engineering and the 1<sup>st</sup> European Early Stage Researchers' Conference on Hydrogen Storage*

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**E 11**

**ELECTRONIC STRUCTURE AND CHARGE TOPOLOGY STUDY OF ALKALI HYDRIDES**

**Bojana Paskaš Mamula, Mirjana Medić, Bojana Kuzmanović,  
Ivana Radisavljević, Nenad Ivanović, Nikola Novaković**

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Electronic structure and Bader charge analysis calculation of alkali hydride series has been performed. Classification of charge topology structures of alkali hydrides within the broader frame of NaCl structures (along with alkali halides) has been established. Additionally, connection between charge topology and experimentally observed trends in macroscopic properties, such as B1-B2 phase transformation pressures, melting points, elastic properties etc., was considered.

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