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**UNIVERZITET CRNE GORE**  
**METALURŠKO-TEHNOLOŠKI FAKULTET**

Podgorica

**PREDMET:** Godišnji izvještaj mentora o napredovanju doktoranda

Poštovani,

U skladu sa Pravilima o izmjenama i dopunama pravila doktorskih studija (Bilten Univerziteta Crne Gore, br. 561 od 04.07.2022. godine), dostavljam Vam Godišnji izvještaj mentora o napredovanju doktoranda MSc Zorane Sekulić.

Srdačan pozdrav,

Mentor

*Asanović*  
Prof. dr Vanja Asanović

Podgorica, 14.09.2022.g.



## GODIŠNJI IZVJEŠTAJ MENTORA O NAPREDOVANJU DOKTORANDA

Akademska godina za koju se podnosi izvještaj	2021/2022				
<b>OPŠTI PODACI O DOKTORANDU</b>					
Titula, ime, ime roditelja, prezime	MSc Zorana Sekulić				
Fakultet	Metalurško-tehnološki fakultet				
Studijski program	Metalurgija i materijali				
Broj indeksa	1/19				
<b>MENTOR/MENTORI</b>					
Mentor	Prof. dr Vanja Asanović	UCG, Crna Gora	Fizička metalurgija		
Ko-mentor	Dr Jasmina Grbović Novaković	Institut za nuklearne nauke „Vinča“, Institut od nacionalnog značaja za Republiku Srbiju, Republika Srbija	Fizička hemija materijala		
<b>EVALUACIJA DOKTORANDA*</b>					
Koliko ste zadovoljni kvalitetom održanih susreta sa doktorandom?	<input type="checkbox"/> 1	<input type="checkbox"/> 2	<input type="checkbox"/> 3	<input type="checkbox"/> 4	<input checked="" type="checkbox"/> 5
(Ako je prethodni odgovor „1“ ili „2“ dati obrazloženje i prijedloge za poboljšanje)					
Da li je definisan plan rada sa doktorandom?	<input checked="" type="checkbox"/> DA <input type="checkbox"/> NE				
Da li je doktorand ostvario napredak prema predviđenom planu rada?	<input checked="" type="checkbox"/> DA <input type="checkbox"/> NE				
(Ako je prethodni odgovor „ne“ dati obrazloženje i prijedloge za poboljšanje)					
Kvalitet napretka doktorandovog istraživačkog rada u periodu za koji se podnosi izvještaj je:	<input type="checkbox"/> 1	<input type="checkbox"/> 2	<input type="checkbox"/> 3	<input type="checkbox"/> 4	<input checked="" type="checkbox"/> 5
(Ako je prethodni odgovor „1“ ili „2“ dati obrazloženje i prijedloge za poboljšanje)					
Ocjena doktorandove spremnosti za konsultacije.	<input type="checkbox"/> 1	<input type="checkbox"/> 2	<input type="checkbox"/> 3	<input type="checkbox"/> 4	<input checked="" type="checkbox"/> 5
Ocjena planiranja i izvršavanja godišnjih istraživačkih aktivnosti i stručnog usavršavanja doktoranda.	<input type="checkbox"/> 1	<input type="checkbox"/> 2	<input type="checkbox"/> 3	<input type="checkbox"/> 4	<input checked="" type="checkbox"/> 5
Ocjena napretka u savladavanju metodologije naučno-istraživačkog rada.	<input type="checkbox"/> 1	<input type="checkbox"/> 2	<input type="checkbox"/> 3	<input type="checkbox"/> 4	<input checked="" type="checkbox"/> 5
Ocjena doktorandovog generalnog odnosa prema studijama.	<input type="checkbox"/> 1	<input type="checkbox"/> 2	<input type="checkbox"/> 3	<input type="checkbox"/> 4	<input checked="" type="checkbox"/> 5
Ocjena ukupnog kvaliteta doktorandovog rada.	<input type="checkbox"/> 1	<input type="checkbox"/> 2	<input type="checkbox"/> 3	<input type="checkbox"/> 4	<input checked="" type="checkbox"/> 5
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\*Ocjene su: 1 – nedovoljan, 2 – dovoljan, 3 – dobar, 4 – vrlo dobar, 5 – odličan



## ISPUNJENOST USLOVA DOKTORANDA

## Spisak radova doktoranda iz oblasti doktorskih studija koje je publikovao doktorand

(dati spisak radova koji sadrži)

Doktorantkinja MSc Zorana Sekulić je rezultate sprovedenog istraživanja predstavila na međunarodnim naučnim konferencijama, a započela je i pripremu rada za objavljivanje u naučnom časopisu sa SCI/SCIE liste. Sljedeći radovi su uspješno predstavljeni na međunarodnim naučnim konferencijama:

1. **Sekulić Z.**, Milanović I., Babić B., Prvulović M., Grbović Novaković J., Asanović V., "Mechanochemical Destabilization of MgH<sub>2</sub>-V Nanocomposites for Hydrogen Storage," Book of Abstracts, *10<sup>th</sup> International Conference of Applied Science*, 25-28 May 2022, Banja Luka, pp. 78.
2. **Sekulić Z.**, Grbović Novaković J., Babić B., Prvulović M., Milanović I., Tošić K., Asanović V., "Hydrogen storage properties of MgH<sub>2</sub>-M (M=Ni, V, Cr) composites," Book of Abstracts, *6<sup>th</sup> International Symposium of Materials for Energy Storage and Conversion mESC-IS 2022*, 5-8 July 2022, Bol, Island of Brac, Croatia.
3. **Sekulić Z.**, Milanović I., Babić B., Prvulović M., Grbović Novaković J., Asanović V., "Mechanochemical synthesis of MgH<sub>2</sub>-V nanocomposites," *Twenty-third Annual Conference YUCOMAT 2022 & Twelfth World Round Table Conference on Sintering WTRCS Program and the Book of Abstracts*, Materials Research Society of Serbia, August 29 – September 2, 2022, Herceg Novi, Montenegro, poster presentation P.S.III.C.14., p. 137.

## Obrazloženje mentora o korišćenju sprovedenih istraživanja u publikovanim radovima

(dati obrazloženje)

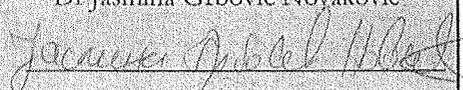
Nakon uspješno sprovedenih eksperimenata, javna odbrana polaznih istraživanja doktorantkinje MSc Zorane Sekulić, pod nazivom: „**Uticaj prelaznih metala na strukturu i sorpcione osobine nanokompozita na bazi magnezijum hidrida**“ održana je 06.12.2021. godine. Odlukom Senata UCG (03-126/1 od 25.01.2022. godine) prihvaćen je Izvještaj Komisije za ocjenu podobnosti doktorske teze i kandidata (obrazac D1).

Doktorantkinja MSc Zorana Sekulić je na međunarodnim konferenciji *10<sup>th</sup> International Conference of Applied Science*, održanoj u maju 2022. godine u Banja Luci (Republika Srpska), predstavila mehanohemijisku destabilizaciju magnezijum hidrida i dopiranje vanadijumom i cilju dobijanja nanokompozita za skladištenje vodonika. Prikazala je rezultate karakterizacije nanokompozitnih sistema pomoću rendgenske strukturne analize (XRD), skenirajuće elektronske mikroskopije (SEM) i infracrvene spektroskopije sa Furijeovom transformacijom (FTIR).

Rezultate analize termijskih promjena uzoraka nanokompozitnih materijala, doktorantkinja MSc Zorana Sekulić je predstavila na međunarodnoj konferenciji *6<sup>th</sup> International Symposium of Materials for Energy Storage and Conversion mESC-IS 2022* održanoj u Republici Hrvatskoj u julu 2022. godine. Primjenom diferencijalne skenirajuće kalorimetrije, analizirani su desorpcioni profili nanokompozita dobijenih destabilizacijom strukture magnezijum hidrida uz dopiranje prelaznim metalima (Ni, V i Cr) u količini od 2 mas % i 5 mas %, pri različitim vremenima mljevenja (15 min, 30 min i 45 min).

Mehanohemijiska sinteza nanokompozita na bazi magnezijum hidrida dopiranog vanadijumom, kao i morfološke i mikrostrukturne promjene, predstavljene su na međunarodnoj konferenciji *Twenty-third Annual Conference YUCOMAT 2022 & Twelfth World Round Table Conference on Sintering WTRCS*, održanoj u Herceg Novom krajem avgusta i početkom septembra 2022. godine. Prikazani



Prikazani su rezultati analize uticaja mehanohemijskih protokola na temperaturu dehidriranja i kinetiku desorpcije vodonika.	
Ocjena o aktivnostima sprovedenim na pisanju i objavljivanju naučnih radova.	<input type="checkbox"/> 1 <input type="checkbox"/> 2 <input type="checkbox"/> 3 <input checked="" type="checkbox"/> 4 <input type="checkbox"/> 5
<b>SAGLASNOST ZA NASTAVAK STUDIJA</b>	
Može li doktorand nastaviti studije?	<input checked="" type="checkbox"/> Da <input type="checkbox"/> Da, uz određene uslove <input type="checkbox"/> Ne
(Ako je prethodno dat odgovor pod „Da, uz određene uslove“ ili „Ne“ dati obrazloženje i prijedloge za poboljšanje)	
<b>Napomene</b>	
(Popuniti po potrebi)	
U Podgorici, 14.09.2022.	
	Prof. dr Vanja Asanović 
	Dr. Jasmina Grbović Noyaković 
MP	

**Prilog dokumenta sadrži:**

- Objavljeni rezultati rada na izradi doktorske disertacije (za drugi izvještaj mentora)





УНИВЕРЗИТЕТ У БАЊОЈ ЛУЦИ  
UNIVERSITY OF BANJA LUKA  
МАШИНСКИ ФАКУЛТЕТ  
FACULTY OF MECHANICAL ENGINEERING



# BOOK OF ABSTRACTS

# 10<sup>th</sup> INTERNATIONAL CONFERENCE OF APPLIED SCIENCE

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# MECHANOCHEMICAL DESTABILIZATION OF $\text{MgH}_2$ -V NANOCOMPOSITES FOR HYDROGEN STORAGE

Z. SEKULIĆ<sup>1</sup>, I. MILANOVIĆ<sup>2</sup>, B. BABIĆ<sup>2</sup>, M. PRVULOVIĆ<sup>2</sup>, J. GRBOVIĆ, NOVAKOVIĆ<sup>2</sup>, V. ASANOVIĆ<sup>3</sup>

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## Abstract

In light of the growing need and necessity for decarbonization, hydrogen plays a decisive role. If hydrogen is aimed to be used as a fuel, the challenges of the low cost of production and safe storage of hydrogen must be overcome. In the current storage methods, hydrogen is compressed under pressure up to 700 bar or liquefied at cryogenic temperatures, i.e., cooling to 20 K (-253,15 °C), meaning high costs and unsafe storage. Therefore, solid-state storage, using primarily metal hydrides, especially light metal hydrides, is a promising solution because it offers safe handling in stationary or mobile applications, as well as higher gravimetric hydrogen capacity. Considering the strong chemical bond between hydrogen and metals in these compounds, which in turn leads to slow kinetics and high dehydration temperatures, the effect of destabilization of the magnesium hydride structure using vanadium as an additive and the method of mechanical milling in a high energy ball mill was examined. The influence on the morphological and microstructural changes in structure was monitored by X-ray diffraction, scanning electron microscopy, particle size analysis and Fourier transform infrared spectroscopy attenuated total reflection. The observed changes were associated with the changes in dehydration temperature and the desorption kinetics of hydrogen followed by DSC analysis. A significant improvement in the performance of the tested material after the applied destabilization methods concerning pure magnesium hydride can be noticed.



# 6<sup>m</sup> ESC-IS 2022

## 6<sup>th</sup> International Symposium on Materials for Energy Storage and Conversion

5. - 8. 7. 2022. Bol, island of Brač, Croatia

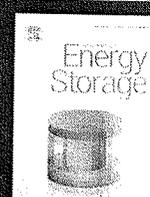
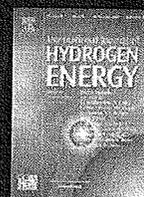
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# BOOK OF ABSTRACTS

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## Hydrogen storage properties of MgH<sub>2</sub>-M (M=Ni,V,Cr) composites

Zorana Sekulić<sup>1</sup>, Jasmina Grbović Novaković<sup>2</sup>, Bojana Babić<sup>2</sup>, Milica Prvulović<sup>2</sup>, Igor Milanović<sup>2</sup>, Katarina Tošić<sup>2</sup>, Vanja Asanović<sup>2</sup>

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The matter of thermodynamic barriers in the decomposition of magnesium hydride is the subject of many scientific studies, primarily through the process of destabilization of the hydride structure [1]. The most commonly used method for hydride destabilization is nanostructuring by mechanical milling which leads to reduction in the particle and crystallite size of the MgH<sub>2</sub> powder. Nanostructuring is often combined with catalyst addition and composite formation [2,3]. Depending on the energy input during the milling process, the typical milling time for magnesium or magnesium hydride ranges from 15 min to 20 h for high-energy mills and from 20 to 150 h for low-energy mills. The most of research is focused on the morphological, structural and thermodynamic effects typical for long milling times, while in this work we have followed the changes taking place under short milling time. The thermal stability of magnesium hydride, is related to structural changes - change of the crystallites and powder particles size. The analysis also considered the changes in activation energy.

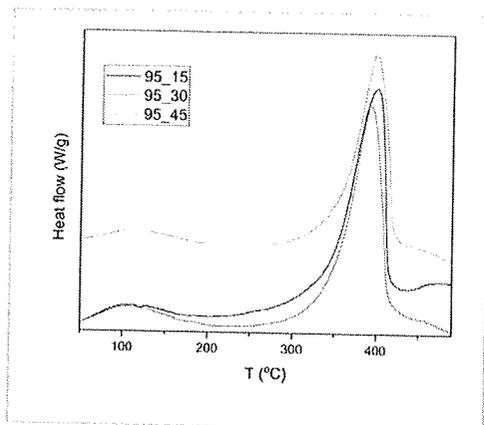


Figure 1. DSC curve for MgH<sub>2</sub>-5% V nanocomposites mechanically milled for 15, 30 and 45 minutes.

MgH<sub>2</sub>-M composites were prepared by mechanical milling of the as-received MgH<sub>2</sub> powder (Alfa Aesar, 98% purity) with the addition of 2 and 5 wt.% of M (M= V, Ni, Cr). Mechanical milling was performed in a SPEX 5100 Mixer Mill using 8mm diameter milling ball. The vial was loaded with powder and balls up to 40% of the volume in order to leave enough space for efficient milling. Samples were milled for 15, 30 and 45 minutes under the inert atmosphere of argon and ball-to-powder ratio 10:1. Figure 1. shows the differential scanning calorimetry (DSC) curves for MgH<sub>2</sub> samples with the addition of 5 wt.% of V milled for 15, (95\_15), 30 (95\_30) and 45 (95\_45) minutes. The DSC curve of commercial powder MgH<sub>2</sub> shows the sharp symmetric high temperature (HT) maximum which originates from desorption from β - MgH<sub>2</sub> at 454°C. The maximum of very low intensity peak is observed at about 350°C, which is a consequence of surface-bound OH groups. If the sample is exposed to the atmosphere, a third, low - temperature maximum may occur, which originates from OH groups and water. It is observed that with increasing milling time hydrogen release temperature increases, which means that shorter milling times have a better effect on the desorption properties of MgH<sub>2</sub>. All three samples show a significantly different desorption profile compared to the commercial sample. The absence of desorption from medium temperatures is clearly visible, but a pronounced low temperature peak (LT) appears at approximately 110 °C.

### References

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- [2] Czujko T, Zaranski Z, Malka IE, Wronski Z. *J Alloy Comp* 509 (2011) S604-7.
- [3] T. Pantić, I. Milanović, M. Lukić, J. Grbović Novaković, S. Kurko, N. Biliškov, S. Milošević Govedarović, *Int. J. Hydrogen Energy* 45(14) (2020) 7901-7911.



Graduate degree in physical chemistry, 1999, Magisterium in physical chemistry, 2003, PhD in physical chemistry 2005. From 1999 works in Vinča Institute of Nuclear Sciences in Laboratory of physics as principal researcher. 2008 Post doc in ENEA CR Casaccia. President of Serbian Society for Microscopy from 2010-2020. 2009 awarded from International Association of Hydrogen Energy with IJHE outstanding Service Award. Guest Editor: *Novel Perspectives on Hydrogen Storage in Solid Media* and *International Journal of Hydrogen Energy*. From 2018 she is the head of Centre of Excellence for Hydrogen and Renewable Energy.  
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Twenty-third Annual Conference  
**YUCOMAT 2022**

&  
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**XII WRTCS**

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and  
**Book of Abstracts**

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**P.S.III.C.13.**

**Electrochemical charge storage properties of thermally treated and ion-beam irradiated graphene oxide/12-tungstophosphoric acid nanocomposites**

Željko Mravik<sup>1</sup>, Marko Gloginjić<sup>1</sup>, Jelena Rmuš<sup>1</sup>, Milica Pejčić<sup>1</sup>, Danica Bajuk-Bogdanović<sup>2</sup>, Maria Vesna Nikolić<sup>3</sup>, Nemanja Gavrilov<sup>2</sup>, Zoran Jovanović<sup>1</sup>

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**P.S.III.C.14.**

**Mechanochemical synthesis of MgH<sub>2</sub>-V nanocomposites**

Z. Sekulić<sup>1</sup>, I. Milanović<sup>2</sup>, B. Babić<sup>2</sup>, M. Prvulović<sup>2</sup>, J. Grbović Novaković<sup>2</sup>, V. Asanović<sup>3</sup>

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**P.S.III.C.15.**

**Structural, optical and mechanical characterization of the PMMA- ZrO<sub>2</sub> nanocomposites**

Ivan Pešić<sup>1</sup>, Miloš Petrović<sup>1</sup>, Dragana Pejić<sup>1</sup>, Maja S. Rabasović<sup>2</sup>, Dragutin Šević<sup>2</sup>, Vesna Radojević<sup>1</sup>

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**YUCOMAT SYMPOSIUM D:**

**ECO-MATERIALS AND ECO-TECHNOLOGIES**

**P.S.III.D.1.**

**Synthesis and characterization of thermally treated geopolymer composite materials**

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**P.S.III.D.2.**

**Photocatalytic activity of N-TiO<sub>2</sub> nanotubes decorated with CdS QD**

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P.S.III.C.14.

### Mechanochemical synthesis of MgH<sub>2</sub>-V nanocomposites

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The future role of hydrogen as an energy vector is inevitable, especially as a basic tool for the decarbonisation of the energy sector. However, in order for hydrogen to gain its full commercial role, challenges such as cost-effective production as well as security of storage must be addressed. Until now, hydrogen was usually stored under pressure (350-700 bar), which poses a significant safety risk or in the liquid state by liquefaction at cryogenic temperatures (-253.15 °C), which implies a high cost of maintaining such low temperatures and the risk of hydrogen leakage. From this point of view, solid state hydrogen storage offers a promising solution both in terms of safety and cost, especially if light metal hydrides are chosen for storage materials. The chemical bond between hydrogen and metals in metal hydrides is usually strong, which in turn leads to slow kinetics and high dehydration temperatures, and it is necessary to cause destabilization of the structure. In this paper, the influence of destabilizing the structure of magnesium hydride using vanadium as an additive and the method of mechanical grinding in a high energy ball mill is investigated.

The influence on the morphological and microstructural changes in structure was monitored by X-ray diffraction, scanning electron microscopy, particle size analysis and Fourier transform infrared spectroscopy attenuated total reflection. Due to the correlation between changes in dehydration temperature and hydrogen desorption kinetics, DSC analysis followed. After applied destabilization methods to pure magnesium hydride, a significant improvement in the performance of the test material is observed.

