

# Bilateral project Serbia-Slovenia (2012/2013)

## Experimental and theoretical investigation of hydrogen sorption in Mg-Zr-Fe-Ni and Ti-Fe-Ni systems

### Project leaders:

Dr Vasil Koteski, Institute Vinča

Dr Andraž Kocjan, Jožef Stefan Institute

### Results of our collaboration so far:

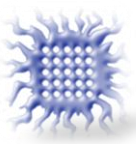
K. Ćirić, A. Kocjan, A. Gradišek, V. Koteski, A. Kalijadis, V. Ivanovski, Z. Laušević, D. Stojić,

*A study on crystal structure, bonding and hydriding properties of Ti-Fe-Ni intermetallics - Behind substitution of iron by nickel*, International Journal of Hydrogen Energy, 37 (2012)8408-8417.

### Future plans...

Mg-Fe-TM, Oxides ...

The project financed by the Ministry of Education and Science,  
Republic of Serbia



## Investigation of intermetallics and semiconductors and possible application in renewable energy sources



**Project leader:** Dr Božidar Cekić (TDPAC, Mossbauer)

- **Members:**
  - Dr Vasil Koteski, (DFT)
  - Dr Dragica Stojić, (Hydrogen sorption investigation)
  - Dr Jelena Belošević-Čavor, (DFT)
  - Dr Ana Umićević, (TDPAC)
  - Valentin Ivanovski, PhD student, (Mossbauer)
  - Jana Radaković, PhD student, (DFT)
  - Katarina Ćirić, PhD student, (Hydrogen storage, DFT)

- **Institution:** **Institute of Nuclear Sciences VINČA**  
Laboratory of Nuclear and Plasma Physics  
Laboratory of Physical Chemistry  
11001 Belgrade, Serbia



# Scientific discipline

## Condensed Matter Physics

### A - Experimental approach:

#### I Nuclear spectroscopy

- Time Differential Perturbed Angular Correlations Spectroscopy (TDPAC)
- Mössbauer Spectroscopy

#### II Hydrogen Sorption Investigations

- Volumetric apparatus
- we expect purchase of PCT apparatus . . .

### B - Computational approach:

#### ➤ Density Functional Theory (DFT)

- Wien2k
- VASP
- Car Parrinello MD

