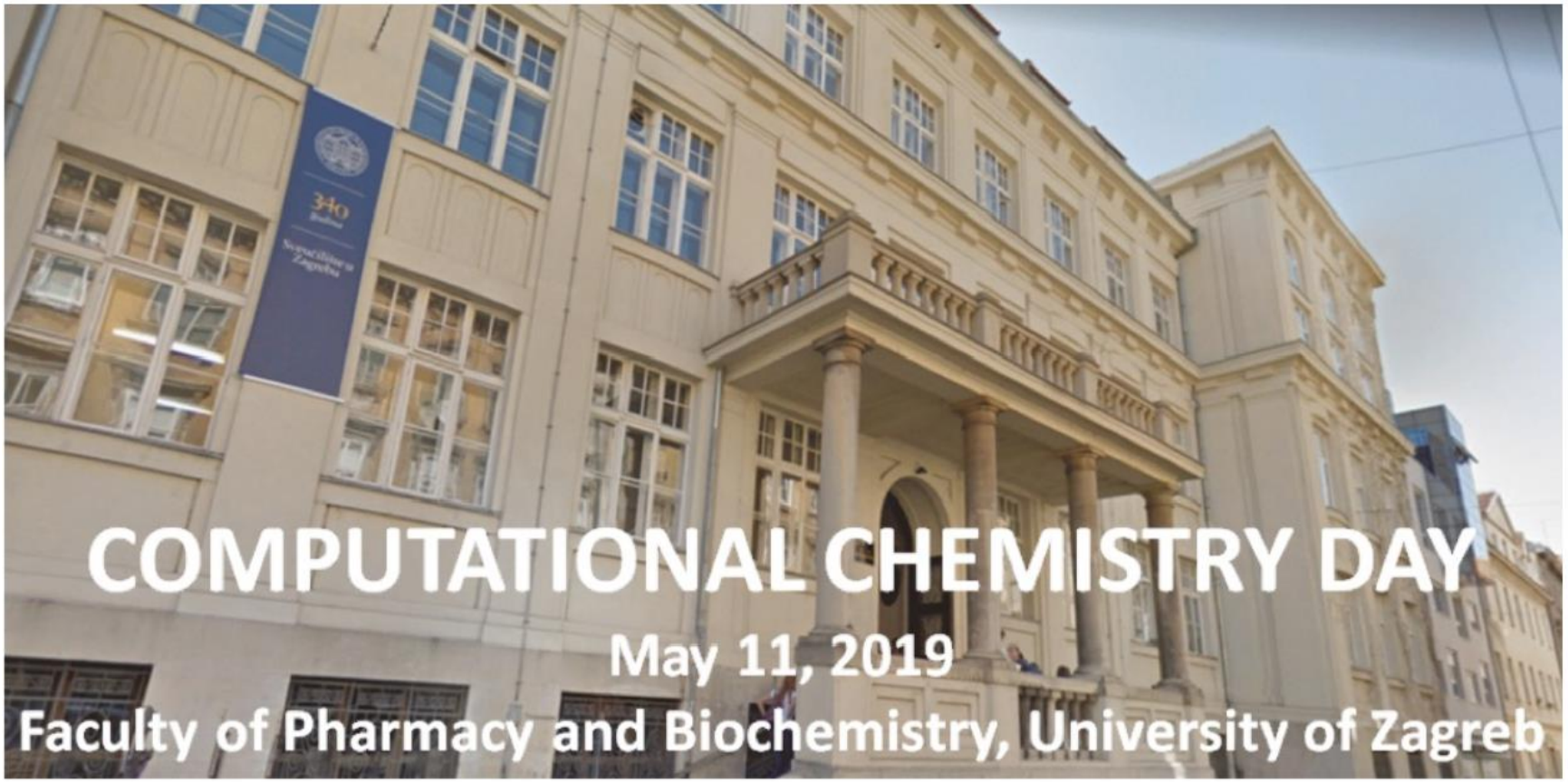
Izvješće o radu

Sekcije za teorijsku i računalnu kemiju HKD

25. 9. 2019.

Computational Chemistry Day



CCD19 Program Participation Organization Sponsors

Computational Chemistry Day

Organizacija:

- **Farmaceutsko – biokemijski fakultet, Sveučilište u Zagrebu**
- **Kemijski odsjek, Prirodoslovno-matematički fakultet, Sveučilište u Zagrebu**
- **Institut Ruđer Bošković, Zagreb**
- **Hrvatsko kemijsko društvo**

Sponzori:

Ministry of Science and Education

HrZZ Croatian Science Foundation

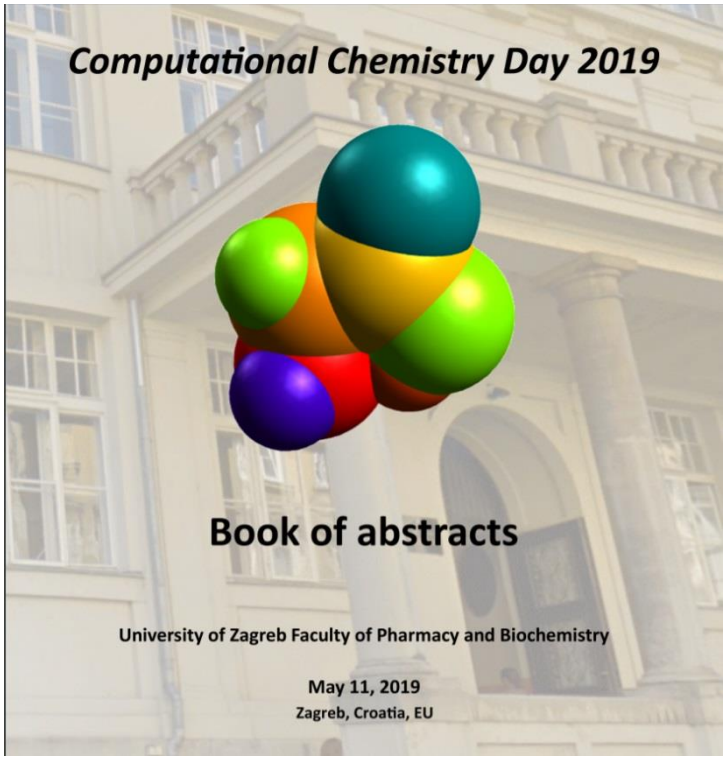
Organizacijski odbor: Darko Babić, Danijela Barić, Marko Cvitaš, Ines Despotović, Nađa Došlić, Marko Hanževački, Mario Vazdar, Tomica Hrenar, Borislav Kovačević, Ivan Ljubić, Zlatko Mihalić, Robert Vianello, Davor Šakić, Valerije Vrček, Tana Tandarić and Tin Weitner

Computational Chemistry Day

- **Uvodna riječ:**

- > 70 učesnika
- 10 predavanja - predavači s različitih institucija (IRB, PMF, FBF, Fidelta, PMF-Split)
- 20 postera

Computational Chemistry Day



2nd Mini symposium on radical enzymes

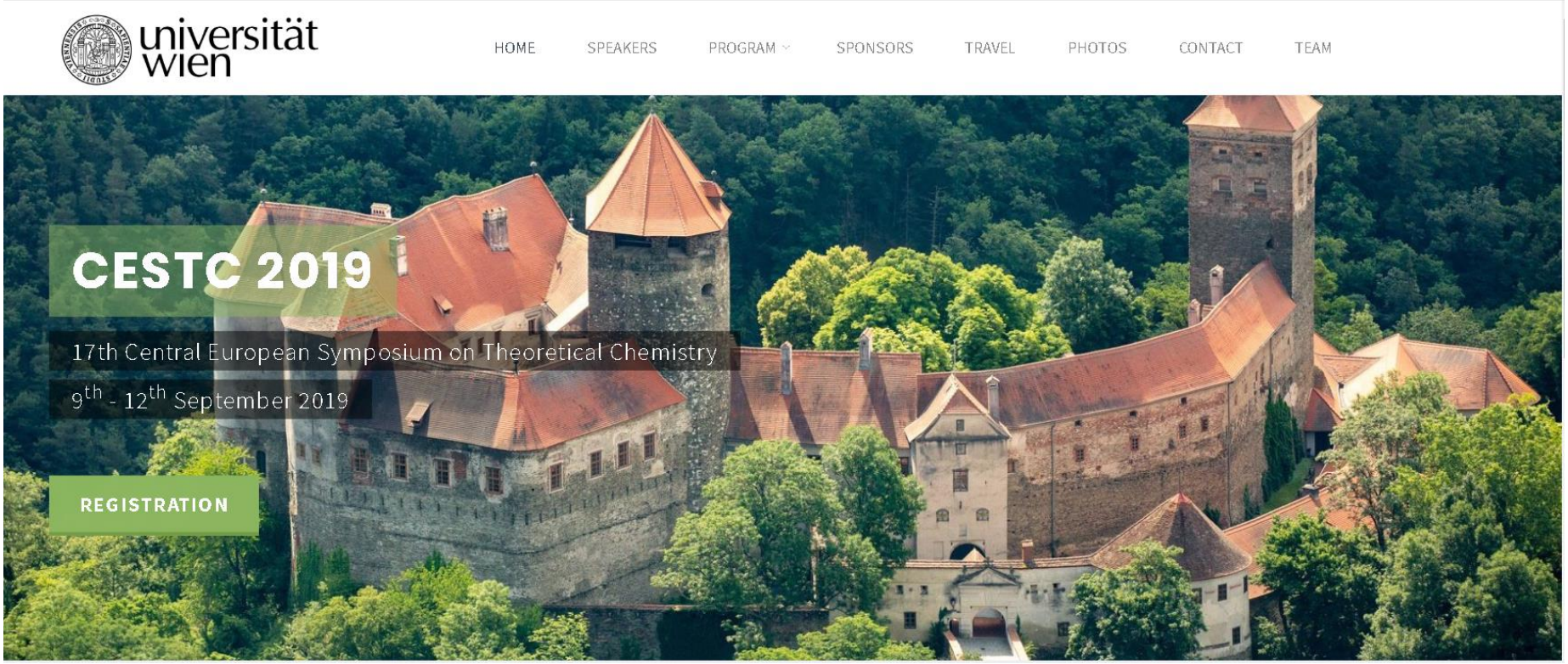
Institut Ruđer Bošković 18. 2. 2019.

Predavač	Naslov predavanja
Dr. Christof Jäger	How nature controls radical and redox chemistry in radical SAM enzymes"
Dr. Gregory M. Sandala	Insight into the Catalytic Mechanism of IspH, an Iron–Sulfur Enzyme in Pathogenic Bacteria, using Broken-Symmetry DFT
Dr. Christian Wick	From Force Fields to QM/MM and back: Modelling chemical change in coenzyme B_{12} dependent enzymes
Luka Bilić, mag. chem	The Role of Enzyme Dynamics in Understanding of Suicidal Inactivation of B_{12}-dependent Diol Dehydratase
Marko Hanževački	Exploring the Stable Conformations during Binding and Unbinding of Coenzyme A in Pyruvate Formate–Lyase

Ostala održana predavanja:

Datum	Predavač/ica	Naslov predavanja
2. 10. 2018.	Dr. Maxim F. Gelin	Enhanced Soret Band Fluorescence from Free base Tetraphenyl-Porphyrin Surface-Mounted Metal Organic Framework: Experiment & Theory
13. 12. 2018.	Dr. Bojan Macan	Plan S i otvoreni pristup znanstvenim publikacijama: jesu li bojazni kemijske zajednice opravdane?
12. 3. 2019.	Dr. Filippo Morini	The ground state nuclear dynamics of dimethyl ether and adamantane in momentum space
19. 3. 2019.	Mag. chem. Robert Stepić	Mechanism of the Water-Gas Shift Reaction in Supported Ionic Liquid Phase
21. 3. 2019.	Dr. Irina Petreska	Conformational switching and electron transport in π-conjugated molecules from first principles: phenylene ethynylene oligomers and more
16. 9. 2018.	Dr. Ivana Gonzales	Design of materials for energy applications guided by computational approaches

CESTC 2019



Czech Republic, Hungary, Poland, Slovakia, Austria and Croatia (from 2019)

Nacionalni predstavnici (Došlić, Hrenar)