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Serbian Chemical Society

University of Belgrade
Faculty of Chemistry

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European Variety in University Chemistry Education

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University Chemistry Education for the Challenges of Contemporary Society

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PREFACE

The conference entitled 7th EuroVariety – European Variety in University Chemistry Education has been organized by the University of Belgrade – the Faculty of Chemistry, the Serbian Chemical Society and the EUCheMS Division of Chemical Education. The main aim of the Conference is to provide an opportunity to share knowledge and experience relating to the important issues concerning university chemistry and chemical technology education in order to prepare future students to better respond to their personal needs and the needs of the contemporary society and to meet the labour market requirements. Therefore, the conference theme "**University Chemistry Education for the Challenges of Contemporary Society**" points out the need for continuous reconsideration of the connections between BSc, MSc and PhD chemistry studies and the contemporary professional, social and scientific challenges.

Over 70 participants from 29 countries have shared their experiences in their presentations offering their insights, pointing up the challenges and suggesting new solutions regarding the following Conference topics:

- Development of the university curricula for BSc, MSc and PhD chemistry studies
- Competency-based university chemistry education
- Chemistry education through university-industry partnerships
- Laboratory work as an element of problem solving and inquiry-based chemistry education
- Ethical guidelines and university chemistry education for sustainable development
- The use of ICT in chemistry education at the 3rd level
- The role of history of chemistry and philosophy of science in university education
- Cultural heritage and chemistry education
- Development of educational competencies of academic chemistry teachers
- Evaluation of learning outcomes and problems relating to assessment in HEIs
- The contemporary chemistry teachers' education and the long-term professional development of chemistry teachers.

Summaries in this Book of Abstracts deal with the practical aspects of teaching chemistry and research into chemistry education at both undergraduate and postgraduate levels with the aim of enabling students to build key professional and transferable skills needed in order to be successful in a highly competitive labour market and life in the rapidly changing world.

I wish all participants a successful conference and fruitful discussion. I hope you will all enjoy your stay in Belgrade.

Dragica Trivic

Head of the Local Organizing Committee

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JIMP 2 SOFTWARE AS A TEACHING TOOL: UNDERSTANDING ORBITALS USING FENSKEE-HALL METHOD

Dušan Ž. Veljković[1], Ivana S. Antonijević[2], and Snežana D. Zarić[1,3]

[1] University of Belgrade – Faculty of Chemistry, Studentski trg 12-16, 11000 Belgrade, Serbia
vdusan@chem.bg.ac.rs

[2] Institute for Chemistry, Technology and Metallurgy, University of Belgrade, Njegoševa 12, 11000 Belgrade, Serbia

[3] Department of Chemistry, Texas A & M University at Qatar, P.O. Box 23874 Doha, Qatar

Teaching molecular orbital concept to undergraduate students is known to be very challenging; analysis of examination data for undergraduate students reveals that they do not have a clear understanding of the concepts of atomic and molecular orbitals (Tsaparlis, 1997). Understanding of the orbital concept has been subject to considerable debate and research (Barradas-Solas and Sánchez Gómez, 2014). One of teaching strategies to deal with this problem is based on usage of different quantum chemical software to calculate shape, energy and to visualize molecular orbitals. The main downside of this approach is the fact that quantum chemical calculations are often very time-consuming, especially in the case of molecules that contain transition metal atoms.

Fenske-Hall method is ab initio method mainly developed for molecular orbitals calculation of transition metal complexes and organometallic compounds (Hall and Fenske, 1972). It was shown that this method is very fast, and very accurate (results are similar to the results obtained by more rigorous and more time-consuming DFT methods).

Here we present a series of computational laboratory exercises using Fenske-Hall method incorporated in Jimp2 software to calculate and visualize both atomic and molecular orbitals. Students will learn how to calculate energy and visualize molecular orbitals of simple molecules. Exercises provide deeper insight into relationship between atomic and molecular orbitals with special emphasis on calculation of contribution of atomic orbitals in particular molecular orbital. Using results of Fenske-Hall calculations, students will construct molecular-orbital diagrams for simple molecules.

Keywords: Orbitals, Fenske-Hall method, Jimp 2

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