

## EDITORIAL

This special issue of *the Journal of the Serbian Chemical Society* is dedicated to Miljenko Perić, Professor Emeritus at the University of Belgrade – Faculty of Physical Chemistry, on the occasion of his 70<sup>th</sup> birthday, in honor of his many achievements in theoretical chemistry, his contribution to university education, and his developing of quantum chemistry and theoretical chemistry at the University of Belgrade.

Miljenko was born in Zagreb on 16 January, 1949. He grew up in Goražde, where his parents were language teachers, and where he finished the high school. He received B.S. (in 1970) and M.S. (in 1974) degrees in physical chemistry at the Faculty of Sciences and Mathematics, University of Belgrade. He stayed at the Institute of Physical Chemistry as a teaching assistant, from 1971 until 1979.

Miljenko's lifelong interest in quantum chemistry began in Germany. Working with Professor Sigrid Peyerimhoff at the Institute for Physical and Theoretical Chemistry at the University of Bonn, he completed in two years, from 1974 to 1976, his doctoral dissertation entitled "Investigation of the Vibrational Structure of Electron Spectra Using the *Ab Initio* Method." At the University of Belgrade he became assistant, associate, and full professor in 1981, 1988 and 1994, respectively. Between the last two dates, the former Faculty of Sciences and Mathematics was divided, and Faculty of Physical Chemistry was established.

Miljenko continued collaborating with Professor Peyerimhoff's research group at the University of Bonn until 2003. He was regularly spending two to three months a year there participating in scientific projects funded by the German Research Foundation, abbreviated DFG. He was a visiting professor at the University of Bonn in 1990–1991, 1998 and 1999; at the Institute for Organic Chemistry of the University of Würzburg in 2004; at the Institute for Theoretical Chemistry at the University of Düsseldorf in 2006; and at the Laboratory for Theoretical Chemistry of the University of Paris-Est in 2007.

As a researcher, Miljenko mostly investigates small linear molecular species with degenerate electronic states. He and his co-workers model the Ren-



ner–Teller effect for linear species containing four, five, six or any number of atoms. They compute vibronic energies for molecules, which cannot be understood without taking into account the non-Born–Oppenheimer effects. Generally, Miljenko mainly applies quantum mechanical *ab initio* procedures in investigating and explaining molecular spectra. Early in his career, Miljenko worked in experimental atomic and molecular spectroscopy and in the physical chemistry of plasma. He is interested also in theoretical chemical kinetics and statistical mechanics.

While publishing more than 160 original papers and reviews, Miljenko also dedicated himself to teaching. He introduced and taught new courses in Physical Chemistry. In the undergraduate and postgraduate curricula, they are Quantum Chemistry, Introduction to the Structure of Matter, and Spectra and Structure. In the doctoral curriculum, they are Theoretical Spectroscopy, Spectroscopy of Polyatomic Molecules, and Application of Group Theory. In his monograph, *Molecular Structure and Molecular Spectra*, published in 2009, Miljenko treats the subjects in more than 1,200 pages. Miljenko led numerous students in their diploma (B.S.) works, M.S. theses, and Ph.D. dissertations. As a member of committees, he selflessly helped students and degree candidates mentored by his colleagues. Miljenko also served as a visiting professor, teaching General Chemistry and Advanced Inorganic Chemistry at the University of Niš, and Atomic Physics at a University of Belgrade branch in Kruševac. At his home institution, in Belgrade, he served as Vice-Dean for teaching in 1988–1991 and 2001–2004.

Students, associates, and colleagues respect Miljenko as a scholar and admire him as a man for his modesty, openness, and selflessness. Miljenko has trained many academics, collaborated with others in research, and influenced large number of students over the decades of his academic career. Some of these students contribute to this Special Issue.

Serbian Academy of Sciences and Arts elected Miljenko as a Corresponding Member in 2003 and as a Full Member in 2009. Serbian Chemical Society gave Miljenko a Medal for his lasting and outstanding contribution to science in 2013. University of Belgrade appointed him Professor Emeritus in 2015.

Miljenko excels also in nonscientific pursuits. As a high-school student, he was the chess champion in Goražde. As a member of a chess club in Bonn, he played in qualifiers for the Bundes League. Still passionate about chess, he is writing commentary of his own chess games. He played recreational football. In consultation with a rabbi, Miljenko translated into Serbian from German, with commentary, a novella by Sholem Aleyhem Shir Hashirim, “A Song of Songs” in 2007.

Miljenko's family is made up of academics. His wife, Jelena, is a retired professor of physical chemistry and university colleague. His son, Ivan, is a professor at Karlsruhe Institute of Technology, Germany.

The papers in this issue deal mostly with theoretical chemistry. Space limits prevented us from inviting contributions by other, equally deserving authors affiliated with Faculties of Physical Chemistry, of Physics, and of Chemistry. We thank all contributors for their efforts, as well as Faculty of Physical Chemistry and Serbian Ministry of Education, Science and Technological Development (Project No. 172040) for financial support.

On behalf of your many colleagues, collaborators and students, we dedicate this Special Issue to you, Miljenko, and hope that you will enjoy it.

Belgrade, August 2019

Guest Editors  
Stanka V. Jerosimić  
Ivan Juranić

Editor-in-Chief  
Branislav Nikolić

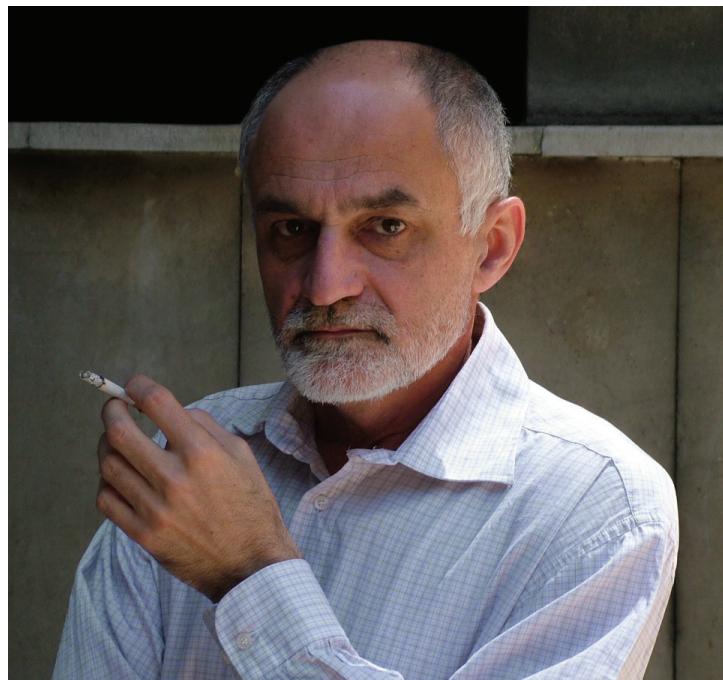
#### SELECTED PUBLICATIONS

- R. J. Buenker, S. D. Peyerimhoff, **M. Perić**, *Ab initio* vibrational analysis of the Schumann-Runge bands and the neighboring absorption region of molecular oxygen, *Chem. Phys. Lett.* **42** (1976) 383.
- M. Perić**, R. Runau, J. Römel, S. D. Peyerimhoff, R. J. Buenker, Calculation of wavefunctions and frequencies for noninfinitesimal vibrations: Comparison of various methods using *ab initio* CI potential curves, *J. Mol. Spectrosc.* **78** (1979) 309.
- R. J. Buenker, **M. Perić**, S. D. Peyerimhoff, R. Marian, *Ab initio* treatment of the Renner-Teller effect for the  $X^2B_1$  and  $A^2A_1$  electronic states of NH<sub>2</sub>, *Mol. Phys.* **43** (1981) 987.
- M. Perić**, S. D. Peyerimhoff, R.J. Buenker, Use of vibronic CI method in accurate calculations of the Renner-Teller effect, *Mol. Phys.* **49** (1983) 379.
- M. Perić**, M. Mladenović, S. D. Peyerimhoff, R. J. Buenker, *Ab initio* study of the isomerization HNC → HCN I. *Ab initio* calculation of the HNC ⇌ HCN potential surface and the corresponding energy levels, *Chem. Phys.* **82** (1983) 317.
- M. Perić**, R. J. Buenker S. D. Peyerimhoff, Theoretical study of the U.V. spectrum of acetylene I. *Ab initio* calculation of singlet electronic states of acetylene by a large-scale CI method, *Mol. Phys.* **53** (1984) 1177.
- M. Perić**, S. D. Peyerimhoff, R. J. Buenker, *Ab initio* treatment of the Renner-Teller effect and application for various AH<sub>2</sub> and HAB molecules“, *Int. Rev.Phys. Chem.* **4** (1985) 85.
- M. Perić**, R. J. Buenker, S. D. Peyerimhoff, *Ab initio* investigation of the vibronic structure of the C<sub>2</sub>H spectrum II. Calculation of diabatic potential surfaces for the three lowest-lying electronic states in C<sub>2</sub>H, *Mol. Phys.* **71** (1990) 673.

- M. Perić**, S. D. Peyerimhoff, R. J. Buenker, *Ab initio* investigation of the vibronic structure of the C<sub>2</sub>H spectrum III. Calculation of vibronic energies and transition probabilities in the X<sup>2</sup>Σ<sup>+</sup>, A<sup>2</sup>Π system, *Mol. Phys.* **71** (1990) 693.
- M. Perić**, S. D. Peyerimhoff, R. J. Buenker, Analysis and predictions of the vibronic spectrum of the ethynil radical C<sub>2</sub>H by *ab initio* methods, *Z. Phys., D* **24** (1992) 177.
- M. Perić**, B. Engels, S. D. Peyerimhoff, Theoretical spectroscopy of small molecules: *Ab initio* investigations of vibronic structure, spin-orbit splitting and magnetic hyperfine effects in the electronic spectra of triatomic molecules, in S.R. Langhoff (Ed): "Quantum Mechanical Electronic Structure Calculations with Chemical Accuracy", Kluwer Academic, Dordrecht, 1995, pp. 261–356.
- M. Perić**, H. Thümmel, C. M. Marian, S. D. Peyerimhoff, *Ab initio* study of the vibronic and spin-orbit coupling in the X<sup>2</sup>Π<sub>u</sub> state of C<sub>2</sub>H<sub>2</sub><sup>+</sup>, *J. Chem. Phys.* **102** (1995) 7142.
- M. Perić**, B. Ostojić, B. Engels, On theoretical model for the Renner-Teller effect in tetraatomic molecules, *J. Chem. Phys.* **105** (1996) 8569.
- C. M. Marian, **M. Perić**, *Ab initio* calculation of the potential energy surface for the large-amplitude bending and symmetric stretching vibration in the electronic ground state of XeF<sub>2</sub>, *Z. Phys. D* **36** (1996) 285.
- C. Pfelzer, M. Havenith, **M. Perić**, P. Mürtz, W. Urban, Faraday laser magnetic resonance spectroscopy of vibrationally excited C<sub>2</sub>H, *J. Mol. Spectrosc.* **176** (1996) 28.
- M. Perić**, B. Ostojić, J. Radić-Perić, *Ab initio* investigation of the Renner-Teller effect in tetra-atomic molecules, *Phys. Reports* **290** (1997) 283.
- M. Perić**, B. Ostojić, B. Schäfer, B. Engels, *Ab initio* treatment of the Renner-Teller effect in tetra-atomic molecules undergoing large amplitude bending vibrations, *Chem. Phys.* **225** (1997) 63.
- M. Perić**, S. D. Peyerimhoff, Rydberg and valence states in tetra-atomic molecules B<sub>2</sub>H<sub>2</sub>, C<sub>2</sub>H<sub>2</sub>, C<sub>2</sub>H<sub>2</sub><sup>+</sup>, in C. Sandorfy (Ed): "Understanding Chemical Reactivity, Vol. 20, The Role of Rydberg states in Spectroscopy and Photochemistry, Low and High Rydberg states", Kluwer Academic, Dordrecht, 1999, pp. 137–174.
- M. Perić**, C. M. Marian, S. D. Peyerimhoff, *Ab initio* study of the vibronic spectrum in the X<sup>2</sup>Π electronic state of HCCS, *J. Chem. Phys.* **114** (2001) 6086.
- M. Perić**, S. D. Peyerimhoff, Renner-Teller effect and spin-orbit coupling in triatomic and tetraatomic molecules, in M. Baer and G. D. Billing (Ed): "The Role of Degenerate States in Chemistry: A Special Volume of Advances in Chemical Physics, Volume 124", Series Editors I. Prigogine and S.A. Rice, John Wiley&Sons, Inc., 2002, pp. 583–658.
- M. Perić**, Theoretical investigations of non-adiabatic effects in molecular spectra, in S.G. Pandalai: "Recent Research Developments in Molecular Spectroscopy", Transworld Research Network, 2002, pp. 177–213.
- M. Perić**, S. D. Peyerimhoff, Perturbative Handling of the Renner-Teller Effect and Spin-Orbit Coupling in Π Electronic States of Triatomic and Tetra-atomic Molecules, *J. Mol. Spectrosc.* **212** (2002) 142.
- C. M. Marian, **M. Perić**, B. Engels, W. Urban, J. M. Brown, Spin-orbit coupling effects in open-shell molecules: The link between theory and experiment, edited by S.D. Peyerimhoff, in "Interactions in Molecules", WILEY-VCH Verlag, Weinheim, 2003, pp. 132–192.
- M. Perić**, Lj. Stevanović, Use of the normal coordinates in variational and perturbative *ab initio* handling of the vibronic and spin-orbit couplings in Π electronic states of linear tetraatomic molecules, *Int. J. Quantum Chem.* **92** (2003) 276.

- M. Perić**, M. Mladenović, B. Engels, An *ab initio* study of the hyperfine structure in the X  $^2\Pi$  electronic state of CCCH, *J. Chem. Phys.* **121** (2004) 2636.
- M. Parac, M. Etinski, **M. Perić**, S. Grimme, A theoretical investigation of the geometries and binding energies of molecular tweezers and clip host-guest systems, *J. Chem. Theory Comput.* **1** (2005) 1110.
- M. Perić**, S. Jerosimić, R. Ranković, M. Krmar, J. Radić-Perić, An *ab initio* model for handling the Renner–Teller effect in tetra-atomic molecules. I. Introduction of coordinates and the Hamiltonian, *Chem. Phys.* **330** (2006) 60.
- M. Perić**, An *ab initio* model for handling the Renner–Teller effect in tetra-atomic molecules. II. Study of the crossing of potential surfaces, *Chem. Phys.* **330** (2006) 73.
- M. Perić**, A model for the Renner–Teller effect in any linear molecule, *Mol. Phys.* **105** (2007) 59.
- M. Perić**, M. Petković, S. Jerosimić, Renner–Teller effect in five-atomic molecules: *Ab initio* investigation of the spectrum of C<sub>5</sub><sup>-</sup>, *Chem. Phys.* **343** (2008) 141.
- M. Perić**, R. Ranković, S. Jerosimić, Renner–Teller effect in six-atomic molecules: *Ab initio* investigation of the vibronic spectrum of C<sub>6</sub><sup>-</sup>, *Chem. Phys.* **344** (2008) 35.
- M. Perić**, Struktura i spektri molekula (engl. *Molecular Structure and Molecular Spectra*), Beograd SANU, 2009, ISBN 978-86-7025-489-3
- R. Vujasin, M. Senčanski, J. Radić-Perić, **M. Perić**, A comparison of various variational approaches for solving the onedimensional vibrational Schrödinger equation, *MATCH* **63** (2010) 363.
- S. Stojadinović, R. Vasilić, M. Petković, I. Belča, B. Kasalica, **M. Perić**, Lj. Zeković, Luminescence during the anodization of zirconium, *Electrochim. Acta* **79** (2012) 133.
- M. Perić**, An alternative derivation of (almost-) Watson's Hamiltonian, *J. Serb. Chem. Soc.* **78** (2013) 1935.
- S. Stojadinović, R. Vasilić, **M. Perić**, Investigation of plasma electrolytic oxidation on valve metals by means of molecular spectroscopy- A review, *RSC Adv.* **4** (2014) 25759.
- M. Perić**, S. Jerosimić, M. Mitić, M. Milovanović, R. Ranković, Underlying theory of a model for the Renner-Teller effect in tetra-atomic molecules: X  $^2\Pi_u$  electronic state of C<sub>2</sub>H<sub>2</sub><sup>+</sup>, *J. Chem. Phys.* **142** (2015) 174306.
- M. Mitić, R. Ranković, M. Milovanović, S. Jerosimić, **M. Perić**, Underlying theory of a model for the Renner–Teller effect in any-atomic linear molecules on example of the X  $^2\Pi_u$  electronic state of C<sub>5</sub><sup>-</sup>, *Chem. Phys.* **464** (2016) 55.
- M. Mitić, M. Milovanović, R. Ranković, S. Jerosimić, **M. Perić**, Topological study of non-adiabatic effects in  $\Pi$  electronic states of tetra-atomic molecules, *Mol. Phys.* **116** (2018) 2671.





### Miljenko Perić – a colleague and a friend for more than half a century

We met as students. I remember him as slender, most often wearing his coffee-colored sweater with a hanger-shaped bulge on the back of his neck. Talkative and humble, intelligent, studious and polite, a great fan of both chess and soccer. That young man grew into a distinguished scientist, professor, and an academician. In my opinion, his main personality trait is the finely tuned sense of balance and justice, which he especially applied to the relationships among people.

Perić's role in the development of the Faculty of Physical Chemistry is well known, but the most important contribution bears repeating: he introduced *quantum chemistry* into the curriculum of our Faculty. Several courses are now based on quantum chemistry, and ten PhD theses have been defended in this area.

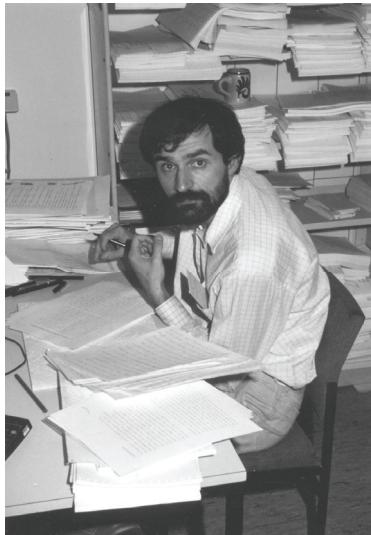
Seven of his former students are now university professors.

Introduction of quantum chemistry was just one of his contributions to the affirmation of our Faculty. I remember his help with the organization of university events, and how he could research and select little-circulated texts related to physical chemistry. These were showcased in 2010 during SANU's commemoration of the centennial of the birth of Prof. Pavle Savić, as well as in 2013, when a grand celebration in the Belgrade City Hall reminded the academic and general audience of the 110<sup>th</sup> anniversary of the instruction of Physical Chemistry at the University of Belgrade.

As an instructor, Miljenko is widely admired and respected by his students. They believed him – as he was always well prepared,

and loved him – as he often engaged them in candid conversations, friendships, soccer matches, or the left-wing political protests he consistently attended. In 2015, I had the pleasure of reporting to the Senate of the University of Belgrade on the work of Prof. Miljenko Perić, on the occasion of his promotion to Professor Emeritus.

Finally, Miljenko and I are as of recently connected through our work on the creation of a book – Š. S. Miljanić, J. Radić-Perić, M. Perić, *Do fisije, o fisiji i o uranijumu* (On Fission and Uranium), Srpska akademija nauka i umetnosti (SANU), Beograd, 2019, in press – which we hope the audience will find interesting; working with him, this book was a pleasure to conceive and write.



Šćepan Miljanić

### **Miljenko Perić as an Adviser to a Charity**

Back in year 2009, I invited Miljenko Perić to join the advisory committee of a fund bearing my name, which gives awards and citations to excellent chemists. Professor Perić accepted the invitation before I finished the sentence. He smoothly integrated himself into this harmonious team of enthusiasts. He worked expertly and diligently. He objectively and astutely evaluated candidates' research accomplishments and merits. He catalyzed agreements.

Professor Perić animated and entertained us with anecdotes and life's experiences; opinions about society and politics; and tidbits about the arts, chess, and football. I nicknamed him Omiljenko ("Dearling" in Serbian). He conscientiously withdrew from the committee in May of 2019, saying that he had enjoyed the work and had felt honored.

We give thanks to Omiljenko for sharing with us his erudition, virtues, and talents. We thank him for bestowing to the fund a part of his prestige. We count on his continued support. All of us are better for having worked with him. Our friendships remain.

Many cheers to Omiljenko!

Nenad M. Kostić