

Branislav Milovanović

Date of birth: 11.10.1993.
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WORKING EXPERIENCE:

August 2018 – Present: **Teaching assistant – University of Belgrade, Faculty of Physical Chemistry**

Subjects (current):

- Statistical Thermodynamics
- Introduction to the Structure of Matter
- Molecular Spectrochemistry
- Chemical Thermodynamics

October 2017 – September 2018: **Physics Teacher – High School „Sveti Sava“**

EDUCATION AND QUALIFICATIONS:

October 2017 – April 2022: **University of Belgrade – Faculty of Physical Chemistry – PhD Studies**

Master thesis: *Theoretical investigation of structure and vibrational spectra of stacked uracil dimers in aqueous solution with Born-Oppenheimer molecular dynamics*

PhD advisor: dr Mihajlo Etinski, Associate Professor

GPA: 10,00 (out of 10,00)

October 2016 – July 2017: **University of Belgrade – Faculty of Physical Chemistry – Master Studies**

Master thesis: *Theoretical investigation of structure and vibrational spectra of stacked uracil dimers in aqueous solution with Born-Oppenheimer molecular dynamics*

Master advisor: dr Mihajlo Etinski, Assistant Professor

GPA: 10,00 (out of 10,00)

October 2012 – July 2016: **University of Belgrade – Faculty of Physical Chemistry – Bachelor Studies**

Bachelor thesis: *Structure and stability of small potassium clusters with iodine*

Bachelor advisor: dr Stanka Jerosimić, Associate Professor

GPA: 9,84 (out of 10,00)

September 2008 – July 2012: **Gymnasium “Miloš Savković”, Department of Mathematics and Science – Aranđelovac, Serbia**

Sep 2000 – Jul 2008 **Primary School – “Milan Ilić Čiča” – Aranđelovac**

RESEARCH EXPERIENCE, COURSES AND SEMINARS:

- July, Sep 2018
Feb 2019;
Jan, Feb 2020;
Sep 2021 Scientific visit to Institute Ruđer Bošković, Zagreb, Croatia to investigate problems concerning photophysics of aqueous dimers of uracil during the project named: „Nonadiabatic transitions of aqueous stacked uracil dimer“ – COST Actions CM1405, CA18222 and CA18212.
- Sep, Oct 2016. Practical training at Lund University, Department of Theoretical Chemistry (*Kemicentrum*), Lund, Sweden – Research of new materials for solar energy conversion using quantum chemical calculations with particular interest in photoexcited properties and electron transfer processes in different light absorbing materials, including dyes with iron and other common metals.

AWARDS:

- 2021 *Studentship for high achievements*, issued by Department of Economy and Social Services of Municipal administration of Aranđelovac, Youth Office, Serbia.
- 2019 *Studentship for high achievements*, issued by Department of Economy and Social Services of Municipal administration of Aranđelovac, Youth Office, Serbia.
- 2018 *Best poster award*, issued by scientific committee of Protein Electrostatics conference held in Belgrade from 25th till 28th June.
- 2018 *Nenad M. Kostić Foundation award for chemical sciences*, cash award for best final year individual project defended on master studies in Republic of Serbia from April the 1st 2017 till the 31st of March 2018.
- 2017 *Serbian Chemical Society special award*, for outstanding overall success during bachelor studies.
- 2017 *Finalist of competition Crown of Success*, organized by family company „Petite Genève Petrović“.
- 2017 *Faculty of physical chemistry award*, for outstanding overall success during studies.
- 2017 *Sister Bulajić Foundation award*, cash award for one of two best final year individual projects defended on bachelor studies of Faculty of physical chemistry, University of Belgrade.
- 2017 *Studentship for high achievements*, issued by Department of Economy and Social Services of Municipal administration of Aranđelovac, Youth Office, Serbia.
- 2016 *Dositeja award for high achievements*, issued by the Fund for Young Talents, Ministry of Youth and Sports of Republic of Serbia.
- 2016 *Studentship for high achievements*, issued by Department of Economy and Social Services of Municipal administration of Aranđelovac, Youth Office, Serbia.
- 2015 *Dositeja award for high achievements*, issued by the Fund for Young Talents, Ministry of Youth and Sports of Republic of Serbia.
- 2014 *Studentship for high achievements during studies*, issued by Ministry of Education, Science and Technological Development of Republic of Serbia.
- 2013 *Studentship for high achievements during studies*, issued by Ministry of Education, Science and Technological Development of Republic of Serbia.
- 2008 *Diploma for outstanding overall success in studying and sports activities*, issued by Primary School „Milan Ilić Čiča“, Aranđelovac, Serbia.

FIELDS OF INTEREST:

Interests:

- Quantum Chemistry
- Molecular Dynamics
- Spectroscopy (Raman, IR, UV/VIS)
- Photophysics and Photochemistry
- Material Science
- Kinetics of Reactions

MEMBERSHIPS:

- Serbian Chemical Society

SKILLS AND TECHNIQUES:

Languages:

- Serbian language – native
- English language – advanced working proficiency
- French language – elementary proficiency

Software skills:

- Gaussian software package – advanced proficiency level
- CP2K software package – advanced proficiency level
- DFTB+ – advanced proficiency level
- OriginLab – advanced proficiency level
- MatLab – intermediate proficiency level
- VMD – intermediate proficiency level
- Siesta software package – intermediate proficiency level
- Quantum Espresso – intermediate proficiency level
- Python programming language – intermediate proficiency level
- LaTeX – intermediate proficiency level
- Turbomole – intermediate proficiency level

PUBLICATIONS:

Marijana Hercigonja, Branislav Milovanović, Mihajlo Etinski, Milena Petković, Decorated Crown Ethers as Selective Ion Traps: Solvent's Role in Crown's Preference Towards a Specific Ion, *J. Mol. Liq.*, **2023**, 381, pp 121791.

<https://doi.org/10.1016/j.molliq.2023.121791>

IF(2021) 6,633

Branislav Milovanović, Jurica Novak, Mihajlo Etinski, Wolfgang Domcke, Nadja Došlić, On the Propensity of Formation of Cyclobutane Dimers in Face-to-Face and Face-to-Back Uracil Stacks in Solution, *Phys. Chem. Chem. Phys.*, **2022**, 24, pp 14836-14845.

<https://doi.org/10.1039/D2CP00495J>

IF(2021) 3,945

Aleksandra Gezović, Jana Mišurović, Branislav Milovanović, Mihajlo Etinski, Jugoslav Krstić, Veselinka Grudić, Robert Dominko, Slavko Mentus, Milica J. Vujković, High Al-ion Storage of Vine Shoots-Derived Activated Carbon: New Concept for Affordable and Sustainable Supercapacitors, *J. Power Sources*, **2022**, 538, pp 231561.

<https://doi.org/10.1016/j.jpowsour.2022.231561>

IF(2021) 9,794

Nemanja Pavković, Branislav Milovanović, Ana Stanojević, Mihajlo Etinski, Milena Petković, Proton leap: Shuttling of Protons onto Benzonitrile, *Phys. Chem. Chem. Phys.*, **2022**, 24, pp 3958-3969.

<https://doi.org/10.1039/D1CP04338B>

IF(2021) 3,945

Branislav Milovanović, Milena Petković, Mihajlo Etinski, Alkaline Earth Cations Binding Mode Tailors Excited-State Charge Transfer Properties of Guanine Quadruplex: A TDDFT Study, *Spectrochim. Acta A*, **2022**, 267 (Part 2), pp 120584.

<https://doi.org/10.1016/j.saa.2021.120584>

IF(2021) 4,831

Branislav Milovanović, Mihajlo Etinski, Igor Popov, Self-Assembly of Rylene-Decorated Guanine Ribbons on Graphene Surface for Optoelectronic Applications: A Theoretical Study, *Nanotechnology*, **2021**, 32 (43), pp 435405.

<https://doi.org/10.1088/1361-6528/ac162c>

IF(2020) 3,874

Branislav Milovanović, Jurica Novak, Mihajlo Etinski, Wolfgang Domcke, Nadja Došlić, Simulation of UV Absorption Spectra and Relaxation Dynamics of Uracil and Uracil-Water Clusters, *Phys. Chem. Chem. Phys.*, **2021**, 23, pp 2594-2604.

<https://doi.org/10.1039/D0CP05618A>

IF(2020) 3,676

Ana Stanojević, Branislav Milovanović, Ivana M. Stanković, Mihajlo Etinski, Milena Petković, The Significance of the Metal Cation in Guanine-Quartet – Metalloporphyrin Complexes, *Phys. Chem. Chem. Phys.*, **2021**, 23, pp 574-584.

<https://doi.org/10.1039/D0CP05798C>

IF(2020) 3,676

Branislav Milovanović, Ivana M. Stanković, Milena Petković, Mihajlo Etinski, Elucidating Solvent Effects on Strong Intramolecular Hydrogen Bond: DFT-MD Study of Dibenzoylmethane in Methanol Solution, *ChemPhysChem*, **2019**, 20 (21), pp 2852-2859.

<https://doi.org/10.1002/cphc.201900704>

IF(2019) 3,144

Branislav Milovanović, Milan Milovanović, Suzana Veličković, Filip Veljković, Aleksandra Perić-Grujić, Stanka Jerosimić, Theoretical and Experimental Investigation of Geometry and Stability of Small Potassium-Iodide K_nI ($n = 2-6$) Clusters, *Int. J. Quantum Chem.*, **2019**, 119 (22), pp e26009.

<https://doi.org/10.1002/qua.26009>

IF(2017) 2,568

Ivana Petrović, Branislav Milovanović, Mihajlo Etinski, Milena Petković, Theoretical Scrutinization of Nine Benzoic Acid Dimers: Stability and Energy Decomposition Analysis, *Int. J. Quantum Chem.*, **2019**, 119 (13), pp e25918.

<https://doi.org/10.1002/qua.25918>

IF(2017) 2,568

Branislav Milovanović, Marko Kojić, Milena Petković, Mihajlo Etinski, New Insight into Uracil Stacking in Water from ab initio Molecular Dynamics, *J. Chem. Theory Comput.*, **2018**, 14 (5), pp 2621–2632.

<https://doi.org/10.1021/acs.jctc.8b00139>

IF(2017) 5,399

Ivana Stanković, Sonja Zrilić, Branislav Milovanović, Ana Stanojević, Milena Petković, Mihajlo Etinski, Binding Symmetric Porphyrins to c-MYC Promoter Pu24I G-quadruplex: Toward More Specific Ligand Recognition by Flanking Bases, *New J. Chem.*, **2023**, Accepted Manuscript.

<https://doi.org/10.1039/D3NJ00956D>

IF(2021) 3,466

Branislav Milovanović, Milena Petković, Igor Popov, Mihajlo Etinski, Water-Mediated Interactions Enhance Alkaline Earth Cation Chelation in Neighboring Cavities of a Cytosine Quartet in the DNA Quadruplex, *J. Phys. Chem. B*, **2021**, 125 (43), pp 11996–12005.

<https://doi.org/10.1021/acs.jpcc.1c05598>

IF(2021) 3,466

Marko Kojić, Igor Lyskov, Branislav Milovanović, Christel Maria Marian, Mihajlo Etinski, The UVA Response of Enolic Dibenzoylmethane: Beyond the Static Approach, *Photochem. Photobiol. Sci.*, **2019**, 17 (6), pp 1324–1332.

<https://doi.org/10.1039/C9PP00005D>

IF(2020) 3,982

Branislav Milovanović, Ivana M. Stanković, Milena Petković, Mihajlo Etinski, Modulating Excited Charge Transfer States of G-Quartet Self-Assemblies by Earth Alkaline Cations and Hydration, *J. Phys. Chem. A*, **2020**, 124 (40), pp 8101–8111.

<https://doi.org/10.1021/acs.jpca.0c05022>

IF(2021) 2,944

Branislav Milovanović, Ana Stanojević, Mihajlo Etinski, Milena Petković, Intriguing Inter-Molecular Interplay in Guanine Quartet Complexes with Alkali and Alkaline Earth Cations, *J. Phys. Chem. B*, **2020**, 124 (15), pp 3002–3014.

<https://doi.org/10.1021/acs.jpcc.0c01165>

IF(2020) 2,991

Branislav Milovanović, Jelica Ilić, Ivana M. Stanković, Milana Popara, Milena Petković, Mihajlo Etinski, A Simulation of Free Radicals Induced Oxidation of Dopamine in Aqueous Solution, *Chem. Phys.*, **2019**, 524, pp 26–30.

<https://doi.org/10.1016/j.chemphys.2019.05.001>

IF(2017) 1,707

Branislav Milovanović, Milena Petković, Mihajlo Etinski, Raman Spectra of Aqueous Uracil Stacked Dimer: First Principle Molecular Dynamics Simulation, *Chem. Phys. Lett.*, **2018**, 713, pp 15–20.

<https://doi.org/10.1016/j.cplett.2018.10.015>

IF(2016) 1,815

Miroslav Ristić, Milena Petković, Branislav Milovanović, Jelena Belić, Mihajlo Etinski, New Hybrid Cluster-Continuum Model for pKa Values Calculations: Case Study of Neurotransmitters' amino Group Acidity, *Chem. Phys.*, **2019**, 516, pp 55–62.

<https://doi.org/10.1016/j.chemphys.2018.08.022>

IF(2016) 1,767

Andjela Simović, Sanja Stevanović, Branislav Milovanović, Mihajlo Etinski, Jelena B. Bajat, Green corrosion inhibitors of steel based on peptides and their constituents: a combination of experimental and computational approach, *J. Solid State Electrochem.*, **2023**, Online Access.

<https://doi.org/10.1007/s10008-023-05433-w>

IF(2021) 2,747

Branislav Milovanović, Milena Petković, Mihajlo Etinski, Properties of the Excited Electronic States of Guanine Quartet Complexes with Alkali Metal Cations, *J. Serb. Chem. Soc.*, **2020**, 85 (8), pp 1021-1032.

<https://doi.org/10.2298/JSC191025140M>

IF(2019) 1,240

Branislav Milovanović, Mihajlo Etinski, Milena Petković, Hydrogen Transfer Reaction: Bond Formation and Bond Cleavage Through the Eyes of Interacting Quantum Atoms, *J. Serb. Chem. Soc.*, **2019**, 84 (8), pp 891-900.

<https://doi.org/10.2298/JSC190226034M>

IF(2019) 1,240

SCIENTIFIC ANNOUNCEMENTS:

Branislav Milovanović, Jurica Novak, Mihajlo Etinski, Wolfgang Domcke, Nađa Došlić, Formation of Cyclobutane Dimers from the Solvated Uracil Stacks, *DEEP-GAS MD-GAS COST Action (CA18212) WG2 & WG3 meeting*, pp 39, Book of Abstracts, Madrid, Spain, October 4-7, **2022**.

Branislav Milovanović, Milica J. Vujković, Mihajlo Etinski, Al³⁺ Cation Interaction with Pristine and Defective Graphene Using Microsolvated Cluster Model: DFT Study, *COIN2022 Contemporary Batteries and Supercapacitors – International Symposium Belgrade 2022*, pp 48, Book of Abstracts ISBN 978-86-82139-86-7, Belgrade, Serbia, June 1-2, **2022**.

Branislav Milovanović, Milena Petković, Mihajlo Etinski, Significant Modulation of Charge-transfer States Properties in the Biological Assembly of the d(TG4T) Sequence in Crystal Form, *Nineteenth Young Researchers' Conference - Materials Science and Engineering*, pp 46, Book of Abstracts ISBN 978-86-80321-36-3, Belgrade, Serbia, December 1-3, **2021**.

Branislav Milovanović, Milena Petković, Mihajlo Etinski, Alkali Metal Cations Impact on the Excited States Properties of the Guanine Quartet, *11th Symposium on Computing π -Conjugated Compounds*, pp 42, Book of Abstracts (<https://cpic-society.com/>), Zagreb, Croatia, January 30 – February 1, **2020**.

Branislav Milovanović, Ivana M. Stanković, Milena Petković, Mihajlo Etinski, Tuning Charge Transfer States in the G-octet-metal Ion Complexes for the Potential Nanotechnological Applications, *Eighteenth Young Researchers' Conference - Materials Science and Engineering*, pp 25, Book of Abstracts ISBN 978-86-80321-35-6, Belgrade, Serbia, December 4-6, **2019**.

Branislav Milovanović, Ivana M. Stanković, Milena Petković, Mihajlo Etinski, Influence of the Metal Ions on the Charge Transfer States in the G-octet-metal Ion Complexes, *Seventh Conference of Young Chemists of Serbia*, pp 153, Book of Abstracts ISBN 978-86-7132-076-4, Belgrade, Serbia, November 2, **2019**.

Branislav Milovanović, Milena Petković, Mihajlo Etinski, Discussing Aqueous Uracil Aggregation with First Principle Molecular Dynamics Simulations, *Sixth Conference of Young Chemists of Serbia*, pp 109-109, Book of Abstracts ISBN 978-86-7132-072-6, Belgrade, Serbia, October 27, **2018**.

Branislav Milovanović, Milan Milovanović, Suzana Veličković, Filip Veljković, Aleksandra Perić-Grujić, Stanka Jerosimić, Ionization Energies of KnI ($n = 2, 3$) Clusters Theoretical and Experimental Evaluation, N-1-P, Physical Chemistry 2018, *14th International Conference on Fundamental and Applied Aspects of Physical Chemistry*, Belgrade, Serbia, Sept 24-28, **2018**.

Branislav Milovanović, Milena Petković, Mihajlo Etinski, On the Importance of π - π Stacking and Hydrogen Bonding Cooperativity on Aqueous Uracil Aggregation, *Protein electrostatics*, pp 59, Book of Abstracts ISBN 978-86-7220-093-5, Belgrade, Serbia, June 25-28, **2018**.

Branislav Milovanović, Milana Popara, Milena Petković, Mihajlo Etinski, *Ab initio* Molecular Dynamics Insights on How Dopamine Disarms Hydroxyl Radical, *55th Meeting of the Serbian Chemical Society*, pp 104, Book of Abstracts ISBN 978-86-7132-069-6, Novi Sad, Serbia, June 8-9, **2018**.

PROJECTS:

- Januar 2020 – Present – Engagement under contracts number 451-03-68/2020-14/200146, 451-03-9/2021-14/200146, 451-03-68/2022-14/200146 and 451-03-47/2023-01/200146 (Faculty of Physical Chemistry, University of Belgrade, Belgrade, Serbia) Ministry of Science, Technological Development and Innovation.
- June 2018 – Januar 2020 – *Structure and dynamics of molecular systems in ground and excited electronic states* (172040, PI dr Mihajlo Etinski, Faculty of Physical Chemistry, University of Belgrade, Belgrade, Serbia) Ministry of Education, Science and Technological Development of Republic of Serbia.
- April 2021 – Present – *Carbon-Based Batteries and Supercapacitors*, SUPERCAR Project NATO SPS G5836 trilateral project (NPD dr Robert Dominko, National Institute for Chemistry, Ljubljana, Slovenia; PPD dr Milica Vujković, Faculty of Physical Chemistry, University of Belgrade, Belgrade, Serbia; Co-Director dr Veselinka Grudić, Faculty of Metallurgy and Technology, University of Montenegro, Podgorica, Montenegro).
- 2020 – 2022 – *Engineering Electronic Properties of Thin-films of Transition Metal Dichalcogenides for Applications in Solar Cells - A Combined Theoretical-Experimental Approach*, bilateral project of Republic of Serbia and Republic of Germany (PI dr Igor Popov, Institute of Physics, Institute of Multidisciplinary Research, Belgrade, Serbia; prof. dr Gianurelio Cuniberti, Institute for Materials Science, TU Dresden, Dresden, Germany).
- 2020 – 2022 – *MXene Nanostructures for Clean Energy Storage Devices*, bilateral project of Republic of Serbia and Republic of France (PI dr Igor Popov, Institute of Physics, Institute of Multidisciplinary Research, Belgrade, Serbia; prof. dr Thomas Niehaus, Institute Lumière Matière, University Claude Bernard, Lyon, France).
- Sep 2016. – Sep 2017 – *Solar Energy Conversion and Catalysis Calculations* (SNIC 2016/1-383) – First principles calculations of molecules and materials which are conducted with a focus on advanced solar energy conversion processes, including dye-sensitized solar cells, artificial photosynthesis, and organic solar cells. The ambition is firstly to provide a better understanding of how solar energy conversion systems function on the molecular level, and secondly to use calculations (mainly DFT and TD-DFT calculations) to guide the search for more efficient molecular components in such systems.