



Curriculum Vitae

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Country of Birth: Serbia

Academic Degree: **1993** B.Sc. Chemistry (*GPA: 9.87 on a 10.0 scale*), Faculty of Chemistry, University of Belgrade
2002 Ph.D. Chemistry (*magna cum laude*), Free University (Freie Universität) of Berlin, Department of Chemistry, Biology and Pharmacy, Germany
dissertation: Modeling of conformation and redox potentials of hemes and other cofactors in proteins

Research Rank: **2007** Assistant Research Professor – Department of Chemistry, University of California, Davis, USA
2015 Associate Research Professor – Institute of Chemistry, Technology and Metallurgy, University of Belgrade, Serbia

Memberships and Academic Service: **2006 – Present** ACS Member (American Chemical Society)

2013 – Present SCS Member (Serbian Chemical Society)

2005 – 2013 Reviewer, Journal of Chemical Thermodynamics (Elsevier)

2006 – Present Reviewer, Journal of Physical Chemistry (ACS)

2013 – Present Reviewer, Journal of Serbian Chemical Society (SCS)

2013 – Present Reviewer, Journals published by Dove Medical Press

2014 – 2018 Reviewer, Nano Letters (ACS)

2020 – Present Reviewer, Photochemical & Photobiological Sciences (Springer)

2020 – Present Reviewer, Frontiers in Chemistry

Professional Experience: **1994 – 1998** Industrial experience, researcher in the Institute for R&D (Lab: Organic synthesis) – Pharmaceutical company *Zdravlje-Actavis*, Leskovac, Serbia

1998 – 2002 Doctoral studies at the Freie Universität, Berlin, Germany

2002 – 2006 Postdoctoral researcher at the University of California, Davis, USA

2007 – 2009 Research Assistant Specialist at the University of California, Davis, USA

2010 – 2011 Study visit at the City College of New York, USA

2011 – 2012 Research Assistant Specialist at the University of California, Davis, USA

2017 Visiting lecturer at UP Diliman, Quezon City, Philippines (Computational methods in biochemistry)

2013 – Present IChTM – Department of Chemistry, University of Belgrade, Serbia

Awards and Honors: **1988 – 1992** Government Undergraduate Scholarship of the Republic of Serbia

1989 – 1993 Scholarship of *ICN-Galenika*, pharmaceutical company

1994 Award of Serbian Chemical Society for the best graduated student in 1992/93 at the Faculty of Chemistry, University of Belgrade

1998 – 2001 Graduate Scholarship, Humboldt University Berlin and German Research Society (DFG)

2001 – 2002 Research Fellowship, Department of Biochemistry - Charité Berlin and DFG (as visiting researcher)

Research Interests:

- Theoretical and computational chemistry
- Computer simulations of biological macromolecules
- Molecular modeling of novel synthetic proteins and chimerical structures
- Molecular mechanics (MM) and molecular dynamics (MD)
- Combined quantum-mechanical/continuum electrostatic approach (QM/MM)
- Electrostatic, pKa and redox-potential calculations
- Bioinformatics and protein data base mining
- Reaction mechanisms in enzymes
- Coupling of electron and proton transfer reactions
- Bioenergetics and kinetics of chemical processes and reactions in proteins

- Proton pumping enzymes
- Cytochromes, membrane proteins, and respiratory electron-transport chain
- DNA photolyases and cryptochromes
- Protein–cofactor/substrate/inhibitor, protein–protein or DNA–protein interactions

- Professional Achievements:**
- Patented new methods of synthesis and characterization of bioactive molecules for treating cardiovascular diseases and scale up for pharmaceutical industrial production
 - Introduced new computational method in research field of theoretical/computational biochemistry and biophysics of biopolymers, such as enzymes, proteins, DNA, polysaccharides, etc. by combining quantum-mechanical and electrostatic calculations
 - Proposed mechanism of proton pumping of cytochrome *c* oxidase – Coulomb pump model with kinetic gating, including gating through conformational states of Glu242 side-chain

Citations: 832 citations, November 2021; h-index = 15 (from Scopus)

Language Skills: Serbian (native), English (proficiency), German (advanced), Russian (basic)

Major Projects: International:

2018 – 2022 COST Action CA17120: "Chemobrionics", Brussels – European Union, Chair of the Action: Prof. Julyan Cartwright (Spain).

2002 – 2012 "Theoretical and computational studies of biological electron transfer", National Institute of Health (NIH grant project, No. GM 054052). Project Director: Prof. Alexei Stuchebrukhov (UC Davis, USA).

2002 – 2012 "Electron tunneling in proteins", National Science Foundation (NSF grant project, No. PHY 0646273). Project Director: Prof. Alexei Stuchebrukhov (UC Davis, USA).

2009 – 2010 "Importance of buried charges in proteins", National Science Foundation (NSF grant project, No. MCB 1022208). Project Director: Prof. Marilyn Gunner (CUNY, USA).

2001 – 2002 "Protein-Kofaktor Wechselwirkungen in biologischen Prozessen", Deutsche Forschungsgemeinschaft (SFB 498). Project Director: Prof. Dietmar Stehlik (Freie Universität Berlin, Germany).

1998 – 2001 "Dynamik und Evolution zellulärer und makromolekularer Prozesse", Deutsche Forschungsgemeinschaft (GRK 268). Project Director: Prof. Reinhart Heinrich (Humboldt Universität Berlin, Germany).

National (Serbian):

2020 – 2021 Financially supported by the Ministry of Education, Science and Technological Development of the Republic of Serbia (MPNTR): Grant No. 451-03-68/2020-14/200026 and 451-03-9/2021-14/200026. The holder of the contract is Institute of Chemistry, Technology and Metallurgy, University of Belgrade.

2013 – 2019 "Rational design and synthesis of biologically active and coordinated compounds and functional materials, relevant in (bio)nanotechnology" (project No. OI/172035, Ministry of Education, Science and Technological Development of the Republic of Serbia). Project Director: Prof. Ivan Jurić.

1994 – 1998 "Exploring new methods of synthesis and semi-synthesis and characterization of bioactive molecules" (project No. 02M34PT3, Ministry of Science and Technology of the Republic of Serbia). Project Director: Dr. Vlastimir Stamenković.

Major Publications: Chapters in distinguished international monographs

1. Quenneville, J., **Popović, D.M.** & Stuchebrukhov, A.A. Chapter 26: Combined Density Functional Theory (DFT) and Electrostatics Study of the Proton Pumping Mechanism in Cytochrome *c* Oxidase. In "Computational Inorganic and Bioinorganic Chemistry", Eds.: E.I. Solomon, R.A. Scott, R.B King. John Wiley & Sons, Ltd., 353-362, **2009**. [ISBN: 978-0-470-69997-3]. This chapter is also available as a part of "Encyclopedia of Inorganic Chemistry", 5-Volume Set (published **2011**). DOI: <https://doi.org/10.1002/0470862106.ia629>
2. **Popović, D.M.**, Quenneville, J. & Stuchebrukhov, A.A. Chapter 3: Combined DFT and Electrostatic Calculations of pK_a 's in proteins: Study of Cytochrome *c* Oxidase. In "Modern Methods for Theoretical Physical Chemistry of Biopolymers", Eds.: E.B. Starikow, J.P. Lewis, S. Tanaka. Elsevier, 53-78, **2006**. [ISBN: 978-0-444-52220-4]. DOI: <https://doi.org/10.1016/B978-044452220-7/50067-8>

Patents

1. Stojanović, N.; Stojičić, S.; Mitov, S.; **Popović, D.** Procedure For Synthesis Of 1,4-Dihydropyridine Derivatives (NIFELAT, NITRENDIPIN, NISOLDIPIN). Application number P-250/99, submitted on 06/04/1999, published on 08/12/2002; Patent number **YU 49947 B**, issued date **09/29/2008**; AD Zdravlje, Center for Research and Development, Vljakova 199, 16000 Leskovac, Yugoslavia.
2. Stojanović, D.; Stanojević, C.; **Popović, D.** Procedure For Synthesis Of Atenolol (ATENOLOL). Application number P-394/98, submitted on 09/07/1998, published on 08/12/2002. Patent number **YU 49569 B**, issued date **04/10/2007**; AD Zdravlje, Center for Research and Development, Vljakova 199, 16000 Leskovac, Yugoslavia.

Journal articles

1. Protić-Rosić, I., Nešić, A., Lukić, I., Miljković, R., **Popović, D.M.**, Atanasković-Marković, M., Stojanović, M., Gavrović-Jankulović M. Recombinant Bet v 1-BanLec chimera modulates functional characteristics of peritoneal murine macrophages by promoting IL-10 secretion, *Molecular Immunology* 138 (2021) 58-67. (<https://doi.org/10.1016/j.molimm.2021.06.015>)
2. **Popović, D.M.** Photolyase – molecular mechanism for repair of UV-damaged DNA. *Hemijski Pregled* 62(3) (2021) 50-62.
3. Lopandić, Z., Dragačević, L., **Popović, D.M.**, Andjelković, U., Minić, R., Gavrović-Jankulović, M.D. BanLec-eGFP chimera as a tool for evaluation of lectin binding to high-mannose glycans on microorganisms, *Biomolecules* 11(2) (2021) article number 180, pp 1-13. (<https://doi.org/10.3390/biom11020180>)
4. **Popović, D.M.**, Djordjević, I. S. Catalytic center of cytochrome c oxidase: Effects of protein environment on pKa values of CuB histidine ligands. *Journal of Serbian Chemical Society* 85 (2020) 1429-1444. (<https://doi.org/10.2298/JSC200720047P>)
5. Lazić, A.M., Djordjević, I.S., Radovanović, L.D., **Popović, D.M.**, Rogan, J.R., Janjić, G.V., Trisović, N.P. Self-assembly and biorecognition of a spirohydantoin derived from α -tetralone: Interplay between chirality and intermolecular interactions. *ChemPlusChem* 85 (2020) 1220-1232. (<https://doi.org/10.1002/cplu.202000273>)
6. Janjić, G.V., Jelić, S.T., Trisović, N.P., **Popović, D.M.**, Djordjević, I.S., Milčić, M.K. New theoretical insight into fluorination and fluorine-fluorine interactions as a driving force in crystal structures. *Crystal Growth & Design* 20 (2020) 2943-2951. (<https://doi.org/10.1021/acs.cgd.9b01565>)
7. Mrkić, I.V., Minić, R.D., **Popović, D.M.**, Zivković, I.P., Gavrović-Jankulović, M.D. Newly designed hemagglutinin-Der p 2 chimera is a potential candidate for allergen specific immunotherapy. *Life Sciences* 213 (2018) 158-165. (<https://doi.org/10.1016/j.lfs.2018.10.036>)
8. **Popović, D.M.** Current advances in research of cytochrome c oxidase. Invited review article, *Amino Acids* 45 (2013) 1073-1087. (<https://doi.org/10.1007/s00726-013-1585-y>)
9. **Popović, D.M.** Nobel prize 2013 for chemistry from the cyber space. *Hemijski Pregled* 53(6) (2013) 142-147.
10. **Popović, D.M.** Cytochrome c oxidase - Molecular proton pump and its reaction mechanism. *Hemijski Pregled* 53(3) (2013) 58-66.
11. **Popović, D.M.**, Stuchebrukhov, A.A. Coupled electron and proton transfer reactions during the O \rightarrow E transition in bovine cytochrome c oxidase. *Biochim. Biophys. Acta-Bioenergetics* 1817 (2012) 506-517. (<https://doi.org/10.1016/j.bbabi.2011.10.013>)
12. Couch, V., **Popović, D.**, Stuchebrukhov, A. Redox-Coupled Protonation of Respiratory Complex I: The Hydrophilic Domain. *Biophys J.* 101 (2011) 431-438. (<https://doi.org/10.1016/j.bpj.2011.05.068>)
13. **Popović, D.M.**, Leontyev, I.V., Beech, D.G., Stuchebrukhov, A.A. Similarity of cytochrome c oxidases in different organisms. *Proteins: Structure, Function, and Bioinformatics* 78 (2010) 2691-2698. (<https://doi.org/10.1002/prot.22783>)
14. Medvedev, E.S., Kotelnikov, A.I., Barinov, A.V., Psikha, B.L., Ortega, J.M., **Popović, D.M.**, Stuchebrukhov, A.A. Protein dynamics control of electron transfer in Photosynthetic Reaction Center from *Rps. Sulfoviridis*.

15. Quenneville, J., **Popović, D.M.**, Stuchebrukhov, A.A. Combined DFT and electrostatics study of the proton pumping mechanism in cytochrome *c* oxidase. *Biochim. Biophys. Acta-Bioenergetics* 1757 (2006) 1035-1046. (<https://doi.org/10.1016/j.bbabi.2005.12.003>)
16. Stuchebrukhov, A.A., **Popovic, D.M.** Comment on "acidity of a Cu-bound histidine in the binuclear center of cytochrome *c* oxidase". *Journal of Physical Chemistry B* 110 (2006) 17286-17287. (<https://doi.org/10.1021/jp057310u>)
17. Makhov, D.V., **Popović, D.M.**, Stuchebrukhov, A.A. Improved density functional theory/electrostatic calculation of the His291 protonation state in cytochrome *c* oxidase: Self-consistent charges for salvation energy calculation. *Journal of Physical Chemistry B* 110 (2006) 12162-12166. (<https://doi.org/10.1021/jp0608630>)
18. **Popović, D.M.**, Stuchebrukhov, A.A. Two conformational states of Glu242 and pKa's in bovine cytochrome *c* oxidase. *Photochemical & Photobiological Sciences* 5 (2006) 611-620. (<https://doi.org/10.1039/b600096g>)
19. **Popović, D.M.**, Quenneville, J., Stuchebrukhov, A.A. DFT/electrostatic calculations of pKa values in cytochrome *c* oxidase. *Journal of Physical Chemistry B* 109 (2005) 3616-3626. (<https://doi.org/10.1021/jp046535m>)
20. **Popović, D.M.**, Stuchebrukhov, A.A. Proton exit channels in bovine cytochrome *c* oxidase. *Journal of Physical Chemistry B* 109 (2005) 1999-2006. (<https://doi.org/10.1021/jp0464371>)
21. Quenneville, J., **Popović, D.M.**, Stuchebrukhov, A.A. Redox-dependent pKa of CuB histidine ligand in cytochrome *c* oxidase. *Journal of Physical Chemistry B* 108 (2004) 18383-18389. (<https://doi.org/10.1021/jp0467797>)
22. **Popović, D.M.**, Stuchebrukhov, A.A. Proton pumping mechanism and catalytic cycle of cytochrome *c* oxidase: Coulomb pump model with kinetic gating. *FEBS Letters* 566 (2004) 126-130. (<https://doi.org/10.1016/j.febslet.2004.04.016>)
23. **Popović, D.M.**, Stuchebrukhov, A.A. Electrostatic study of the proton pumping mechanism in bovine heart cytochrome *c* oxidase. *Journal of the American Chemical Society* 126 (2004) 1858-1871. (<https://doi.org/10.1021/ja038267w>)
24. **Popović, D.M.**, Zmirić, A., Zarić, S.D., Knapp, E.W. Energetics of radical transfer in DNA photolyase. *Journal of the American Chemical Society* 124 (2002) 3775-3782. (<https://doi.org/10.1021/ja016249d>)
25. **Popović, D.M.**, Zarić, S.D., Knapp, E.W. Factors determining the orientation of axially coordinated imidazoles in heme proteins. *Biochemistry* 40 (2001) 7914-7928. (<https://doi.org/10.1021/bi010428q>)
26. **Popović, D.M.**, Zarić, S.D., Rabenstein, B., Knapp, E.W. Artificial cytochrome *b*: Computer modeling and evaluation of redox potentials. *Journal of the American Chemical Society* 123 (2001) 6040-6053. (<https://doi.org/10.1021/ja003878z>)
27. Zarić, S.D., **Popović, D.M.**, Knapp, E.W. Metal ligand aromatic cation- π interactions in metalloproteins: Ligands coordinated to metal interact with aromatic residues. *Chemistry - A European Journal* 6 (2000) 3935-3942. ([https://doi.org/10.1002/1521-3765\(20001103\)6:21<3935::AID-CHEM3935>3.0.CO;2-J](https://doi.org/10.1002/1521-3765(20001103)6:21<3935::AID-CHEM3935>3.0.CO;2-J))
28. **Popović, D.M.** New theoretical insight into protein environment – redox properties relationship in synthetic mono-heme proteins. *Inorganic Chemistry*, (2022), to be published.

Selected presentations and conference papers

1. **D. Popović**, "Proton pumping mechanism of cytochrome *c* oxidase: Electron-coupled proton transfer reactions" *Invited Talk*, Gordon Research Conference "Protons & Membrane Reactions", Ventura, CA, USA, February 22-27, 2009.
2. **D. Popović**, A. Stuchebrukhov, "Coupled electron transfer: Proton transfer reactions and proton pumping mechanism of cytochrome *c* oxidase" *Invited Talk*, ACS Symposium in honor of Rudolph Marcus "Fifty Years of Electron Transfer and RRKM Theories" at 232nd American Chemical Society National Meeting, San

Francisco, CA, USA, September 10-14, **2006**.

3. N.P. Trišović, S.T. Jelić, **D.M. Popović**, I.S. Đorđević, M.K. Milčić, G.V. Janjić, "The Fluorination as a Driving Force in Crystal Structures" *Poster*, Quantum Crystallography Online Meeting - QCrOM2020, Paris, France, August 26-29 **2020**.
4. **D. Popović**, I. Juranić, "Influence of protein environment on redox properties of cofactors: Redox potentials of artificial cytochrome *b*" *Conference paper & Talk*, Proceedings, pp. 96-100 (TH O1), 52nd Meeting of the Serbian Chemical Society, Novi Sad, Serbia, May 29-30, **2015**.
5. **D. Popović**, "Photoactivation mechanism of DNA photolyase" *Talk*, 8th International Conference of the Chemical Societies of the South-East European Countries (ICOSEC 8), Belgrade, Serbia, June 27-29, **2013**.
6. **D. Popović**, "Energetics of the steps in proton pumping mechanism and preventing of backflow reactions in cytochrome *c* oxidase" *Talk*, 8th International Conference of the Chemical Societies of the South-East European Countries (ICOSEC 8), Belgrade, Serbia, June 27-29, **2013**.
7. **D.M. Popović**, V. Medaković, S.D. Zarić, E.W. Knapp, "Factors determining the orientation of axially coordinated imidazoles in heme model systems and heme-proteins" *Conference paper*, Eds.: S. Ribnikar, S. Anić. Physical Chemistry 2000, Proceedings of the 5th International Conference on Fundamental and Applied Aspects of Physical Chemistry (2000), pp. 339-342, Belgrade, Yugoslavia, September 27-29, **2000**.
8. **D. Popović**, E.W. Knapp, "Calculating redox potential in native and artificial cytochrome *b*" *Poster*, 3rd European Biophysics Conference 2000, München, Germany, September 9-13, **2000**.
9. **D. Popović**, E.W. Knapp, "Artificial Metallo-Proteins – A Model of Cytochrome *b*" *Poster*, 5th World Congress of Theoretically Oriented Chemists, WATOC-99, London, UK, August 1-6, **1999**.