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Laboratorija za teorijsku hemiju

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**Elektronska pošta:** dpopovic@chem.bg.ac.rs

**Obrazovanje:** 1993. Diplomirani hemičar, Hemijski fakultet, Univerzitet u Beogradu.

2002. Doktor hemijskih nauka, Freie Universität, Berlin, Nemačka.

**Zvanja:** 2007. Assistant Specialist, step III, (Naučni saradnik) na University of California, Davis

2013. Istraživač saradnik

2015. Viši naučni saradnik

**Članstva u društvima:** Srpsko hemijsko društvo, Američko hemijsko društvo

**Profesionalno iskustvo:** 1994 – 1998 Istraživač u Institutu za istraživanje i razvoj – Farmaceutska kompanija *Zdravlje* Leskovac

1998 – 2002 Doktorske studije na Freie Universität, Berlin, Nemačka

2002 – 2006 Postdoktorske studije na University of California, Davis, SAD

2006 – 2008 Naučni saradnik (Assistant Specialist) na University of California, Davis, SAD

2009 – 2010 Studijski boravak na City College of New York, SAD

2011 – 2012 Naučni saradnik na University of California, Davis, SAD

2013 – IHTM – Centar za hemiju

- Oblasti interesovanja:**
- Teorijska i računarska hemija
  - Komjuterske simulacije bioloških makromolekulekula
  - Molekulsko modelovanje
  - Molekulska mehanika i molekulska dinamika
  - Kombinovani kvantno-mehanički/kontinuum elektrostatički proračuni (QM/MM)
  - Pretraga proteinske baze podataka
  - Proračuni pKa vrednosti amino-kiselinskih ostataka i redoks potencijala kofaktora u proteinima
  - Reakcioni mehanizami enzima
  - Sprezanje reakcija transfera elektrona i protona
  - Bioenergetika hemijskih procesa u proteinima
  - Kinetika hemijskih reakcija
  - Membranski proteini i protonske pumpe
  - Respiratorni electron-transportni niz

**Znanje jezika:** Engleski i Nemački

**Najznačajniji projekti: Međunarodni:**

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

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

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

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

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

#### Osnovna istraživanja:

**2013 – 2015** "Racionalni dizajn i sinteza biološki aktivnih i koordinacionih jedinjenja i funkcionalnih materijala, relevantnih u (bio)nanotehnologiji" (projekat br. OI/172035, Ministarstvo za nauku i tehnološki razvoj Republike Srbije). Rukovodilac projekta: Dr. Aleksandar Nikolić.

#### Primenjena istraživanja:

**1994 – 1998** "Istraživanje novih postupaka sinteze i polusinteze i karakterizacija bioaktivnih molekula" (projekat br. 02M34PT3, Ministarstvo za nauku i tehnologiju Republike Srbije). Rukovodilac projekta: Dr. Vlastimir Stamenković.

#### Izabrane publikacije: Poglavlja u istaknutnim monografijama međunarodnog značaja:

1. **Popović, D.M.**, Quenneville, J., Stuchebrukhov, A.A. Chapter 3/ Combined DFT and Electrostatic Calculations of pKa'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]
2. **Popović, D.M.**, Quenneville, J., 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.: Edward I. Solomon, Robert A. Scott, Bruce R. King. John Wiley & Sons, Ltd., 353-362, **2009**. [ISBN: 978-0-470-69997-3]

#### Publikovani radovi:

1. Zarić, S.D., **Popović, D.M.**, Knapp, E.W. Metal ligand aromatic cation- $\pi$  interactions in metalloproteins: Ligands coordinated to metal interact with aromatic residues. *Chemistry - A European Journal* 6 (**2000**) 3935-3942.
2. **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.
3. **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.
4. **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.
5. **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.
6. **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.
7. **Popović, D.M.**, Stuchebrukhov, A.A. Proton exit channels in bovine cytochrome *c* oxidase. *Journal of*

*Physical Chemistry B* 109 (2005) 1999-2006.

8. Quenneville, J., **Popović, D.M.**, Stuchebrukhov, A.A. Redox-dependent p*K*<sub>a</sub> of CuB histidine ligand in cytochrome *c* oxidase. *Journal of Physical Chemistry B* 108 (2004) 18383-18389.
9. **Popović, D.M.**, Quenneville, J., Stuchebrukhov, A.A. DFT/electrostatic calculations of p*K*<sub>a</sub> values in cytochrome *c* oxidase. *Journal of Physical Chemistry B* 109 (2005) 3616-3626.
10. **Popović, D.M.**, Stuchebrukhov, A.A. Two conformational states of Glu242 and p*K*<sub>a</sub>'s in bovine cytochrome *c* oxidase. *Photochemical & Photobiological Sciences* 5 (2006) 611-620.
11. 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.
12. **Popović, D.M.**, Quenneville, J., 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.
13. 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*. *Journal of Physical Chemistry B* 112 (2008) 3208-3216.
14. **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.
15. Couch, V., **Popović, D.**, Stuchebrukhov, A. Redox-Coupled Protonation of Respiratory Complex I: The Hydrophilic Domain. *Biophys J.* 101 (2011) 431-438.
16. **Popović, D.M.**, Stuchebrukhov, A.A. Coupled electron and proton transfer reactions during the O→E transition in bovine cytochrome *c* oxidase. *Biochim. Biophys. Acta-Bioenergetics* 1817 (2012) 506-517.
17. **Popović, D.M.** Citohrom *c* oksidaza - Molekulska proton pumpa i njen reakcioni mehanizam. *Hemijski Pregled* 53, br.3 (2013) 58-66.
18. **Popović, D.M.** Nobel Prize 2013 for Chemistry from the cyber space. *Hemijski Pregled* 53, br.6 (2013) 142-147.
19. **Popović, D.M.** Current Advances in Research of Cytochrome *c* Oxidase. Invited review article, *Amino Acids*, 45 (2013) 1073-1087.

#### Saopštenja:

1. **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 232<sup>nd</sup> American Chemical Society National Meeting, San Francisco, CA, USA, September 10-14, 2006.
2. **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.
3. **D. Popović**, E.W. Knapp, "Artificial Metallo-Proteins – A Model of Cytochrome *b*." 5<sup>th</sup> World Congress of Theoretically Oriented Chemists, WATOC-99, London, UK, August 1-6, 1999.
4. **D. Popović**, E.W. Knapp, "Calculating redox potential in native and artificial cytochrome *b*." 3<sup>rd</sup> European Biophysics Conference 2000, München, Germany, September 9-13, 2000.
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. Popović**, I. Juranić, “Influence of protein environment on redox properties of cofactors: Redox potentials of artificial cytochrome *b*.” *Conference paper & Talk*, Vol: Proceedings, pp. 96-100 (TH O 1), 52nd Meeting of the Serbian Chemical Society, Novi Sad, Serbia, May 29-30, 2015.
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**Dragan M. Popović**

**Viši naučni saradnik**