



# Dr Sonja Grubišić

## Viši naučni saradnik

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**Obrazovanje:** 1997 Diplomirani hemičar, Hemijski fakultet, Univerzitet u Beogradu

2001 Magistar hemijskih nauka, Hemijski fakultet, Univerzitet u Beogradu

2005 Doktor hemijskih nauka, Hemijski fakultet, Univerzitet u Beogradu

**Zvanja:** 2002 Istraživač saradnik

2006 Naučni saradnik

2012 Viši naučni saradnik

**Nagrade i priznanja:** 2008 Stipendija Univerziteta u Padovi (Institut za nuklearnu fiziku-Galileo Galilej) za postdoktorsko usavršavanje

2011 Stipendija Univerziteta u Pisi (Scuola Normale Superiore) za postdoktorsko usavršavanje

**Clanstva u društvima:** Srpsko hemijsko društvo, Italijansko hemijsko društvo

**Profesionalno iskustvo:** 2002- IHTM – Centar za hemiju,

1999-2006 Hemijski fakultet, Univerzitet u Beogradu

**Oblasti interesovanja:** Teorijska hemija, teorijska fizika, koordinaciona hemija, hemija čvrstog stanja, medicinska hemija, fizika kondenzovane materije

**Znanje jezika:** Srpski (maternji), Engleski, Italijanski

**Najznačajniji projekti:** Međunarodni:

2008-2010 PRIN Nacionalni projekat Italije.

2011– 2014 CMST COST Action CM1002 (Convergent Distributed Environment for Computational Spectroscopy). Evropska unija (Brisel, Belgija). MC member.

2012 PSTC-1 (Computational design of materials displaying room temperature magnetic bistability). Ministarstvo prosvete i nauke RS (Beograd); Ministry of Science and Innovation of the Kingdom of Spain (Madrid, Španija).

2013-2015 Bilateralni projekat između Republike Srbije i Republike Italije ( Computational study of bio- and nano-systems: chemical, spectroscopic and conformational aspects). Ministarstvo prosvete i nauke RS (Beograd),

Jedinica za nauku i tehnologiju Ministarstva spoljnih poslova Republike Italije. Rukovodilac srpskog projektnog tima.

**2015-2019** CMST COST Action CM1405 (Molecules in motion). Evropska unija (Brisel, Belgija). MC member, STSM coordinator.

#### **Osnovna istraživanja:**

**2001-2005** 101569 (Hemijske i biohemijske konsekvence metal ligand interakcija). Ministarstvo za nauku Republike Srbije (Beograd).

**2006-2010** 142017 (Hemijske i biohemijske konsekvence metal ligand interakcija). Ministarstvo za nauku Republike Srbije (Beograd).

**2011-** 172035 (Racionalni dizajn i sinteza biološki aktivnih i koordinacionih jedinjenja i funkcionalnih materijala, relevantnih u (bio) nanotehnologiji). Ministarstvo za nauku i tehnološki razvoj Republike Srbije (Beograd).

- Izabrane publikacije:**
1. Tamara Todorović, Sonja Grubišić, Matej Pregelj, Marko Jagodič, Sonja Misirlić-Denčić, Marija Dulović, Ivanka Marković, Olivera Klisurić, Aleksandar Malešević, Dragana Mitić, Katarina Anđelković and Nenad Filipović, **Structural, magnetic, DFT and biological studies of mononuclear and binuclear Cu(II) complexes with bidentate N-heteroaromatic Schiff base ligand**. European Journal of Inorganic Chemistry (2015) 23, 3921-3931.
  2. Sonja Grubišić, Svetozar Niketić, **Potential energy surface evaluation and fitting**. Reference Module in Chemistry, Molecular Sciences and Chemical Engineering (2015).
  3. Ivana Djordjevic, Sonja Grubišić, Miloš Milčić, Svetozar Niketić, **Derivation of a new set of force field parameters for ammine complexes of chromium(III) containing halogeno ligands: modeling the trans-influence of halogenido ligands**. JOURNAL OF THE SERBIAN CHEMICAL SOCIETY (2015) 80 (3) 329-342.
  4. Nenad Filipović, Sonja Grubišić, Maja Jovanović, Marija Dulović, Ivanka Marković, Olivera Klisurić, Aleksandar Marinković, Dragana Mitić, Katarina Anđelković, Tamara Todorović, **Palladium(II) complexes with N-heteroaromatic bidentate hydrazon ligands: the effect of the chelate ring size and lipophilicity on in vitro cytotoxic activity**. CHEMICAL BIOLOGY & DRUG DESIGN (2014) 84 (3) 331-341.
  5. S. Grubišić, G. Brancato and V. Barone, **An improved AMBER force field for  $\alpha, \alpha$  dialkylated peptides: intrinsic and solvent-induced conformational preferences of model systems**. PHYSICAL CHEMISTRY CHEMICAL PHYSICS (2013), 15 (48) 17395-17407.
  6. Sonja Grubišić, Giuseppe Brancato, Alfonso Pedone, Vincenzo Barone, **Extension of the AMBER force field to cyclic  $\alpha, \alpha$  dialkylated peptides**. PHYSICAL CHEMISTRY CHEMICAL PHYSICS (2012), 14 (44) , 15308-20.
  7. Pier Luigi Silvestrelli, Alberto Ambrosetti, Sonja Grubisic, Francesco Ancilotto **Adsorption of rare-gas atoms on Cu(111) and Pb(111) surfaces by van der Waals-corrected density functional theory**. PHYSICAL REVIEW B (2012), 85, 165405.
  8. Marko Peric, Matija Zlatar, Sonja Grubisic, Maja Gruden-Pavlovic, **Magnetic couplings mediated through the non-covalent interactions**, POLYHEDRON (2012), 42, 89-94.
  9. Anđelković Ljubica, Perić Marko, Zlatar Matija, Grubišić Sonja, Gruden- Pavlović Maja, **Magnetic criteria of aromaticity in benzene cation and benzene anion: How does the Jahn-Teller effect influence the aromaticity?** TETRAHEDRON LETT. (2012), 53 (7) , 794-799.
  10. Perić Marko, Zlatar Matija, Gruden-Pavlović Maja, Grubišić Sonja, **DFT study of the magnetic coupling interaction in a series of binuclear oxalate complexes**. MONATSCHEFTE FUR CHEMIE-CHEMICAL MONTHLY (2012), 143 (4) 569-577.

11. Ancilotto Francesco, Da Re Marco, [Grubišić Sonja](#), Hernando Alberto, Silvestrelli Pier Luigi, Toigo Flavio, **Grand Canonical Monte Carlo study of argon adsorption in aluminium nanopores.** MOLECULAR PHYSICS (2011), 109, 2787-279.
12. Perić Marko, Niketić Svetozar, Zlatar Matija, Gruden-Pavlović Maja, [Grubišić Sonja](#), **DFT and MM Description of the Structure and Magnetic Properties of Manganese Complexes with X-phenylcyanamido Bridging Ligand.** MONATSCHEFTE FÜR CHEMIE-CHEMICAL MONTHLY (2011), 142(6), 585-592.
13. Andjelković Ljubica; [Grubišić Sonja](#); Djordjević Ivana; Zlatar Matija; Niketić Svetozar R.; Gruden-Pavlović Maja, **Consistent force field for metalloporphyrins** JOURNAL OF THE SERBIAN CHEMICAL SOCIETY (2010), 75, 1671-1683.
14. Da Re Marco; [Grubišić Sonja](#); Ancilotto Francesco, **Monte Carlo Simulations of Argon adsorption in nanoscopic linear channels.** PHYS. REV. B (2010), 81, 205427.
15. Silvestrelli Pier Luigi; Benyahia Karima; [Grubišić Sonja](#); Ancilotto Francesco; Toigo Flavio, **Van der Waals interactions at surfaces by density functional theory using Wannier functions.** THE JOURNAL OF CHEMICAL PHYSICS (2009), 130 (7), 074702.
16. [Grubišić Sonja](#); Gruden-Pavlović Maja; Radanović Dusanka D., Perić Marko, Niketić Svetozar R., **Molecular mechanics description of the stabilized effects in (ethylenediamine- N,N'-diacetato)chromate(III) dinuclear complex bridged by pyrazole-3,5-dicarboxylate: DFT calculations of magnetic properties,** JOURNAL OF MOLECULAR STRUCTURE (2009), 919(1-3), 54-58.
17. Gruden-Pavlović Maja; [Grubišić Sonja](#); Zlatar Matija; Niketić Svetozar R., **Molecular mechanics study of nickel(II) octaethylporphyrin adsorbed on graphite(0001).** INTERNATIONAL JOURNAL OF MOLECULAR SCIENCES (2007), 8(8), 810-829.
18. [Grubišić Sonja](#); Radanović Dusanka D.; Rychlewska Urszula; Warzajtis Beata; Drašković Nenad S. ; Miloš Djuran I.; Niketić Svetozar R. **Conformational study of Co(II), Ni(II) and Cr(III) complexes of the EDTA-type: Crystal structure of 1D polymeric *trans*(O<sup>6</sup>)-Ba[Co(1,3-pddap)]·8H<sub>2</sub>O complex stabilized by infinite water tapes.** POLYHEDRON (2007), 26(13), 3437-3447.
19. [Grubišić Sonja](#); Gruden-Pavlović Maja; Niketić Svetozar R.; Sakagami-Yoshida Narumi; Kaizaki Sumio, **Structural analysis of conformational flexibility in (aqua)(propanediamine-N,N'-diacetato-N-propionato)chromium(III) dihydrate. Crystal structure of cis-polar, *trans*(H<sub>2</sub>O,O<sup>5</sup>)-[Cr(1,3-pddap)(H<sub>2</sub>O)] · 2H<sub>2</sub>O.** JOURNAL OF COORDINATION CHEMISTRY (2007), 60(8), 851-863.
20. [Grubišić Sonja](#); Milčić Miloš K.; Radanović Dusanka D.; Niketić Svetozar R., **Conformational analysis of edta-type rhodium(III) complexes with mixed five- and six-membered chelate rings. Structural analysis of conformational flexibility in rhodium(III) complexes containing 1,3-propanediamine-N,N'-diacetate-N,N'-di-3-propionate ligand.** JOURNAL OF MOLECULAR STRUCTURE (2006), 794(1-3), 125-132.
21. [Grubišić Sonja](#); Niketić Svetozar R.; Radanović Dusanka D.; Rychlewska Urszula; Warzajtis Beata, **Layered crystal structure of the *trans*(O<sub>5</sub>O<sub>6</sub>) isomer of potassium (1,3- propanediamine-N,N'-diacetato-N,N'-di-3-propionato)cobaltate(III) trihydrate, *trans*(O<sub>5</sub>O<sub>6</sub>)-K[Co(1,3-pddap)]·3H<sub>2</sub>O, stabilized by ionic, hydrogen bond and CO dipolar interactions: Conformational analysis of Co(III) complexes with the 1,3-propanediamine-N,N'-diacetate-N,N'-di-3-propionate ligand.** POLYHEDRON (2005), 24(13), 1701-1709.
22. Gruden-Pavlović Maja; [Grubišić Sonja](#); Niketić Svetozar R. **Conformational analysis of octa- and tetrabromo tetraphenylporphyrins and their Ni(II) and Tb(III) complexes.** JOURNAL OF INORGANIC BIOCHEMISTRY (2004), 98(8), 1293-1302.
23. [Grubišić Sonja](#); Gruden-Pavlović Maja; Niketić Svetozar R.; Kaizaki Sumio; Sakagami-Yoshida Narumi, **Structural characterization and conformational analysis of (aqua)(ethylenediamine-N,N,N'-triacetato)chromium(III) monohydrate complex. Crystal structure of the *cis*-equatorial isomer of [Cr(ed3a)(H<sub>2</sub>O)]·H<sub>2</sub>O.** INORGANIC CHEMISTRY COMMUNICATIONS (2003), 6(9), 1180-1184.
24. [Grubišić Sonja](#); Gruden-Pavlović, Maja; Niketić Svetozar R.; Sakagami-Yoshida Narumi; Kaizaki Sumio, **Structural characterization of the *trans*-equatorial isomer of (aqua)(ethylenediamine-N,N,N'-triacetato)chromium(III) trihydrate, [Cr(edtrp)(H<sub>2</sub>O)]·3H<sub>2</sub>O.** TRANSITION METAL CHEMISTRY

(2003), 28(1), 37-42.

25. Grubišić Sonja; Gruden Maja; Niketić Svetozar R.; Sakagami-Yoshida Narumi; Kaizaki Sumio, **Conformational analysis of EDTA-type chromium(III) complexes with  $\beta$ -propionato metal chelate rings**. JOURNAL OF MOLECULAR STRUCTURE (2002), 609(1-3), 1-9.

26. Gruden Maja; Grubišić Sonja; Niketić Svetozar R.; Coutsolelos A. G., **Conformational analysis of octa- and tetrahalogenated tetrahenylporphyrins and their metal derivatives**. JOURNAL OF MOLECULAR STRUCTURE (2001), 595(1-3), 209-224.

### **Knjige i revijalni radovi:**

1. Gruden-Pavlović Maja, Grgurić-Šipka Sanja, Grubišić Sonja, Niketić Svetozar R., **Laboratory Practicum for General Chemistry**, Faculty of Chemistry, Belgrade, (2008).

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