Grubišić M. Sonja
(Research Professor)

PERSONAL DATA

Name: Grubišić Sonja

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ACADEMIC BACKGROUND

1997	BSc in Chemistry, University of Belgrade, Serbia
2001	MSc in Computational Chemistry, University of Belgrade
2005	PhD in Computational Chemistry, University of Belgrade

FELLOWSHIPS AND AWARDS

2008	Post-doctoral fellowship, Department of Physics " Galileo Galilei ", University of Padova, Italy
2011	Post-doctoral fellowship, Scuola Normale Superiore, University of Pisa, Italy

MEMBERSHIPS OF SCIENTIFIC SOCIETIES

Serbian Chemical Society, Italian Chemical Society (2013)

SCIENTIFIC DUTIES

2021 Guest Editor of the Frontiers in Chemistry

TEACHING ACTIVITIES

1999-2006 Teaching assistant in the field of Computational Chemistry, General

and Inorganic Chemistry, Solid State Chemistry and Coordination Chemistry at Department of Inorganic Chemistry, University of Belgrade

supervised PhD theses: 2

ORGANISATION OF SCIENTIFIC MEETINGS

Aug 2017 Chair of the Local Organizing Comittee of the Joint Training School of the COST Actions CM1401 Our Astrochemical History and CM1405 MOLIM: Molecules in Motion entitled: New Avenues in molecular theories: From the lab to beyond the Eart, Belgrade, Serbia.

PROJECTS:

International:

2008-2010 PRIN Padova, Italy

2011– 2014 CMST COST Action CM1002 (Convergent Distributed Environment for Computational Spectroscopy). European Union (Brussels, Belgium). MC member

2012 PSTC-1 (Computational design of materials displaying room temperature magnetic bistability). Ministry of education and Science of Republic of Serbia ; Ministry of Science and Innovation of the Kingdom of Spain (Madrid, Špain)

2013-2015 Bilateral Serbian-Italian Project (Computational study of bio- and nano-systems: chemical, spectroscopic and conformational aspects). Ministry of education and Science of Republic of Serbia, Ministry for Foreign Affairs of Republic of Italy. Serbian principal investigator

2015-2019 CMST COST Action CM1405 (Molecules in motion). European Union (Brussels, Belgium). MC member, STSM coordinator

2018-2022 COST Action CA17120 Chemobrionics, European Union (Brusseles, Belgium). MC member.

2021-2025 Confined Molecular Systems: The new generation of materials, Madrid, Spain. Project member from Serbia.

Basic research:

2001-2005 Chemical and biochemical consequences of metal-ligand interactions. Grant number 101569. Ministry of Science of the Republic of Serbia (Belgrade)

2006-2010 Chemical and biochemical consequences of metal-ligand interactions. Grant number 142017. Ministry of Science of the Republic of Serbia (Belgrade)

2011- Rational design and synthesis of biologically active and coordination compounds and functional materials, relevant for (bio)nanotechnology. Grant numbers 172035, 451-03-

68/2020-14/200026 and 451-03-9/2021-14/200026. Ministry of education and Science of Republic of Serbia (Belgrade)

PROGRAMMING EXPERIENCE in Fortran

SOFTWARES GAUSSIAN, AMBER, NAMD, Quantum-ESPRESSO, GROMACS, ORCA, RASPA **,** SIESTA, LAMMPS

LANGUAGES Serbian, English, Italian (basic knowledge)

Representative publications

1. Silvestrelli Pier Luigi, Benyahia Karima, **Grubisic Sonja,** Ancilotto Francesco, Toigo Flavio, *The Journal of Chemical Physics* (2009) 130 (7) 074702-4. DOI: 10.1063/1.3077288.
2. Ancilotto Francesco, Da Re Marco, **Grubisic Sonja**, Hernando Alberto, Silvestrelli Pier Luigi,Toigo Flavio, *Molecular Physics* (2011) 109 2787-279. DOI:10.1080/00268976.2011.610369.
3. Pier Luigi Silvestrelli, Alberto Ambrosetti, **Sonja Grubisic,** Francesco Ancilotto, *Physical Review B* (2012) 85 165405-11. DOI: 10.1103/physrevb.85.165405.
4. **Sonja Grubišić,** Giuseppe Brancato, Alfonso Pedone, Vincenzo Barone, *Physical Chemistry Chemical Physics* (2012) 14 (44) 15308-20. DOI:10.1039/c2cp42713c.
5. **S. Grubišić,** G. Brancato and V. Barone, *Physical Chemistry Chemical Physics* (2013) 15 (48) 17395-17407. DOI: 10.1039/c3cp52721b.
6. **Grubišić Sonja**, Chandramouli Balasubramanian, Barone Vincenzo, Brancato Giuseppe, *Physical Chemistry Chemical Physics* (2016) 18 20389-20398. DOI: 10.1039/C6CP01120A.
7. H. Elshaflu, T. Todorović, M. Nikolic, A. Lolic, A. Visnjevac, S. Hagenow, J. M.Padron, A. T. Garcia-Sosa, I. Djordjević, S. Grubišić, H. Stark and N. Filipović, *Frontiers in Chemistry* (2018) 6: 247. DOI:10.3389/fchem.2018.00247.
8. R. Dahmani, **S. Grubišić,** S. Ben Yaghlane, S. Boughdiri, M. Hochlaf, *J. Phys. Chem. A* (2019)123 (26) 5555-5565. DOI: 10.1021/acs.jpca.9b03228.
9. T. T. Adejumo, N. V. Tzouras, L. P. Zorba, D. Radanović, A. Pevec, **S. Grubišić,** D. Mitić , K. K. Anđelković, G. C.Vougioukalakis, B. Čobeljić, I. Turel, *Molecules* (2020) 25 (18) 4043. DOI: 10.3390/molecules25184043.
10. R. Dahmani, **S. Grubišić**, I. Djordjevic, S. Ben Yaghlane, S. Boughdiri, G. Chambaud, M. Hochlaf, *J. Chem. Phys.* (2021) 154 (2) 024303-10. DOI: 10.1063/5.0037594.
11. M. Jovanovic, N.Turkovic, B. Ivkovic, Z. Vujic, K. Nikolic, **S. Grubisic,** *Structural Chemistry* (2021) 32 2341-2353.DOI:10.1007/s11224-021-01810-1.

BOOKS AND REVIEWS

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