

Name and Surname: Stevan Armaković
Date of Birth: 07.09.1985.
Address: Vaska Pope 3/11, Novi Sad
Phone: +381/63-10-19-036
E mail: stevan.armakovic@df.uns.ac.rs
Web Site: www.armakovic.com



Working Experience

- **2010 – present**, University of Novi Sad, Faculty of Sciences, Department of Physics
Assistant Research Professor
Duties:
 - Research of various molecules, ionic liquids and nanostructures applying DFT calculations and molecular dynamics simulations
 - Teaching activities in Biophysics related courses for students of Physics, Chemistry and Biology
 - Teaching activities in course of Qualitative methods in Physics
 - Participation in activities related to the popularization of science (Design and administration of the web site dedicated to the activities in CERN)
 - Guest lecturer at Petnica research center

Education

- **PhD in Theoretical Physics of Condensed Matter, Molecular Modeling (2014)**, University of Novi Sad, Faculty of Sciences, Department of Physics
- **Graduated Physicist (2009)**, University of Novi Sad, Faculty of Sciences, Department of Physics
- **Music School (2000)**, Sremska Mitrovica – Instrument clarinet

Rewards and Certificates

- **COOL scientist – Researcher Night (2016)**, University of Novi Sad
- **Reward at the 8th Young Researchers Conference for the best oral presentation (2011)**, organized by Materials Research Society of Serbia
- **Utrecht Summer School (16-27. 08. 2010.)** course “Theoretical Physics”, University of Utrecht, Netherlands
- **Reward of the University of Novi Sad (2010)**, for the accomplished results during studies
- **Third prize at republic competition for young clarinetists (1998)**, Belgrade, Ministry of Education
- **Third prize at republic competition for young clarinetists (1997)**, Belgrade, Ministry of Education

Research Interests

Density Functional Theory (DFT) calculations and molecular dynamics (MD) investigation of:

- organic molecules and nanostructures
- graphene, nanotubes and buckybowls
- ionic liquids

- drugs and organometallic molecules
- adsorption properties
- molecular transport, single molecule junctions and photovoltaic
- advanced oxidation processes

Languages

English – advanced level, German – ground level

Experience in Molecular Modeling Software/Code

- **Schrödinger Materials Science Suite**
- **Quantum Wise Virtual Nanolab, Atomistix Toolkit**
- **Amsterdam Density Functional Molecular Modeling Suite**
- **Gaussian 03/09**
- **GAMESS**

Other computational skills

- **Mathematical languages:** Mathematica, Matlab
- **Statistical analysis of results:** Origin Lab
- **Web Design:** Serif Web Plus
- **OS:** Ubuntu, Windows

Research Grants

- **2015 – present**
Support by Schrödinger Inc, license for Materials Science Modeling Suite
- **2011 – present**
Design and modeling of specific properties of nanostructures
Grant no. OI 171 039, Ministry of Education, Science and Technological Development of the Republic of Serbia – researcher
- **2011 – present**
Improvement of forensic methods and their application Grant no. TR 34019, Ministry of Education, Science and Technological Development of the Republic of Serbia – researcher
- **2010 – 2011**
Improvement of physical properties of nanostructured materials - Ministry of Education, Science and Technological Development of the Republic of Serbia - researcher

Reviews

Verified reviewer at Publons - <https://publons.com/author/459312/stevan-armakovic#profile>

- Has reviewed for 13 journals
- 27 Pre-Publication Reviews
- Reviewed for journals:
 - ACS Applied Materials & Interfaces
 - Journal of Molecular Modeling
 - Physics Letters A

- International Journal of Quantum Chemistry
- International Journal of Hydrogen Energy
- Zeitschrift für Naturforschung A
- Computational Materials Science
- Journal of Physical Chemistry
- Arabian Journal of Chemistry
- Journal of Computer-Aided Molecular Design
- Acta Physica Polonica A
- Journal of Alloys and Compounds
- Heliyon

Publications

Top 5 publications:

1. **Stevan Armaković**, Sanja J. Armaković, Slawomir Koziel
OPTOELECTRONIC PROPERTIES OF CURVED CARBON SYSTEMS
Carbon 111 (2017) 371-379, (IF: 6.198)
2. **Stevan Armaković**, Sanja J. Armaković, Svetlana Pelemiš, Dragoljub Mirjanić
INFLUENCE OF SUMANENE MODIFICATIONS WITH BORON AND NITROGEN ATOMS TO ITS HYDROGEN ADSORPTION PROPERTIES
Physical Chemistry Chemical Physics 18 (2016) 2859-2870, (IF: 4.493)
3. **Stevan Armaković**, Sanja J. Armaković, Milan Vraneš, Aleksandar Tot, Slobodan Gadžurić
DETERMINATION OF REACTIVE PROPERTIES OF 1-BUTYL-3-METHYLIMIDAZOLIUM TAURATE IONIC LIQUID EMPLOYING DFT CALCULATIONS
Journal of Molecular Liquids 222 (2016) 796-803, (IF: 2.740)
4. Sanja J. Armaković, **Stevan Armaković**, Nina L. Finčur, Filip Šibul, Davide Vione, Jovan P. Šetrajić, Biljana F. Abramović
INFLUENCE OF ELECTRON ACCEPTORS ON THE KINETICS OF METOPROLOL PHOTOCATALYTIC DEGRADATION IN TiO₂ SUSPENSION. A COMBINED EXPERIMENTAL AND THEORETICAL STUDY
RSC Advances 5 (2015) 54589-54604, (IF: 3.840)
5. **Stevan Armaković**, Sanja J. Armaković, Jovan P. Šetrajić
HYDROGEN STORAGE PROPERTIES OF SUMANENE
International Journal of Hydrogen Energy 38 (2013) 12190-12198, (IF: 4.054)

Rest of publications:

6. Renjith Raveendran Pillai, Vidya V Menon, Shyma Y Mary, C. Yohannan Panicker, **Stevan Armaković**, Sanja J. Armaković
VIBRATIONAL SPECTROSCOPIC INVESTIGATIONS, MOLECULAR DYNAMIC SIMULATIONS AND MOLECULAR DOCKING STUDIES OF N'-DIPHENYLMETHYLIDENE-5-METHYL-1H-PYRAZOLE-3-CARBOHYDRAZIDE
Journal of Molecular Structure 1130 (2017) 208-222, (IF: 1.780)
7. Javeed Ahmad War, K. Jalaja, Y. Sheena Mary, C. Yohannan Panicker, **Stevan Armaković**, Sanja J. Armaković, Santosh Kumar Srivastava, Christian Van Alsenoy
SPECTROSCOPIC CHARACTERIZATION OF 1-[3-(1H-IMIDAZOL-1-YL)PROPYL]-3-PHENYLTHIOUREA AND ASSESSMENT OF REACTIVE AND OPTOELECTRONIC PROPERTIES EMPLOYING DFT CALCULATIONS AND

MOLECULAR DYNAMICS SIMULATIONS

Journal of Molecular Structure 1129 (2017) 72-85, (IF: 1.780)

8. Vidya V. Menon, Egemen Foto, Y. Sheena Mary, Esin Haratas, C. Yohannan Panicker, Gözde Yalcin, **Stevan Armaković**, Sanja J. Armaković, C. Van Alsenoy, Ilkay Yildiz
VIBRATIONAL SPECTROSCOPIC ANALYSIS, MOLECULAR DYNAMICS SIMULATIONS AND MOLECULAR DOCKING STUDY OF 5-NITRO-2-PHENOXYMETHYL BENZIMIDAZOLE
Journal of Molecular Structure 1129 (2017) 86-97, (IF: 1.780)
9. Y. Sheena Mary, Nourah Z. Alzoman, Vidya V. Menon, Ebtehal S Al-Abdullah, Ali A. El-Emam, C. Yohannan Panicker, Ozlem Temiz-Arpaci, **Stevan Armaković**, Sanja J. Armaković, Christian Van Alsenoy
REACTIVE, SPECTROSCOPIC AND ANTIMICROBIAL ASSESSMENTS OF 5-[(4-METHYLPHENYL) ACETAMIDO]-2-(4-TERT-BUTYLPHENYL)BENZOXAZOLE: COMBINED EXPERIMENTAL AND COMPUTATIONAL STUDY
Journal of Molecular Structure 1128 (2017) 694-706, (IF: 1.780)
10. D. Alwani Zainuri, Suhana Arshad, N. Che Khalib, I. Abdul Razak, Renjith Raveendran Pillai, S. Fariza Sulaiman, N. Shafiqah Hashim, K. Leong Ooi, **Stevan Armaković**, Sanja J. Armaković, C. Yohannan Panicker, C. Van Alsenoy
SYNTHESIS, XRD CRYSTAL STRUCTURE, SPECTROSCOPIC CHARACTERIZATION (FT-IR, ¹H AND ¹³C NMR), DFT STUDIES, CHEMICAL REACTIVITY AND BOND DISSOCIATION ENERGY STUDIES USING MOLECULAR DYNAMICS SIMULATIONS AND EVALUATION OF ANTIMICROBIAL AND ANTIOXIDANT ACTIVITIES OF A NOVEL CHALCONE DERIVATIVE, (E)-1-(4-BROMOPHENYL)-3-(4-IODOPHENYL)PROP-2-EN-1-ONE
Journal of Molecular Structure 1128 (2017) 520-533, (IF: 1.780)
11. K. Jalaja, Y. Sheena Mary, C. Yohannan Panicker, **Stevan Armaković**, Sanja J. Armaković, B.K. Sagar, M. Girisha, H.S. Yathirajan, Christian Van Alsenoy
SPECTROSCOPIC CHARACTERIZATION OF 4-[2-(5-ETHYLPYRIDIN-2-YL)ETHOXY]BENZALDEHYDE OXIME AND INVESTIGATION OF ITS REACTIVE PROPERTIES BY DFT CALCULATIONS AND MOLECULAR DYNAMICS SIMULATIONS
Journal of Molecular Structure 1128 (2017) 245-256, (IF: 1.780)
12. **Stevan Armaković**, Sanja J. Armaković, Biljana F. Abramović
THEORETICAL INVESTIGATION OF LORATADINE REACTIVITY IN ORDER TO UNDERSTAND ITS DEGRADATION PROPERTIES: DFT AND MD STUDY
Journal of Molecular Modeling 22 (2016) 240, (IF: 1.438)
13. Fatmah A.M. Al-Omary, Y. Sheena Mary, Shargina Beegum, C. Yohannan Panicker, Mona M. Al-Shehri, Ali A. El-Emam, **Stevan Armaković**, Sanja J. Armaković, Christian Van Alsenoy
MOLECULAR CONFORMATIONAL ANALYSIS, REACTIVITY, VIBRATIONAL SPECTRAL ANALYSIS AND MOLECULAR DYNAMICS AND DOCKING STUDIES OF 6-CHLORO-5-ISOPROPYLPYRIMIDINE-2,4(1H,3H)-DIONE, A POTENTIAL PRECURSOR TO BIOACTIVE AGENT
Journal of Molecular Structure 1127 (2017) 427-436, (IF: 1.780)
14. Vidya V. Menon, Edakot Fazal, Y. Sheena Mary, C. Yohannan Panicker, **Stevan Armaković**, Sanja J. Armaković, Subban Nagarajan, Christian Van Alsenoy
FT-IR, FT-RAMAN AND NMR CHARACTERIZATION OF 2-ISOPROPYL-5-METHYLCYCLOHEXYL QUINOLINE-2-CARBOXYLATE AND INVESTIGATION OF ITS REACTIVE AND OPTOELECTRONIC PROPERTIES BY MOLECULAR DYNAMICS SIMULATIONS AND DFT CALCULATIONS
Journal of Molecular Structure 1127 (2017) 124-137, (IF: 1.780)

15. **Stevan Armaković** and Sanja J. Armaković
INVESTIGATION OF BORON MODIFIED GRAPHENE NANOSTRUCTURES;
OPTOELECTRONIC PROPERTIES OF GRAPHENE NANOPARTICLES AND
TRANSPORT PROPERTIES OF GRAPHENE NANOSHEETS
Journal of Physics and Chemistry of Solids 98 (2016) 156-166, (IF: 2.048)
16. Berta Barta Hollo, József Magyari, **Stevan Armaković**, Goran Bogdanović, Marko Rodić,
Sanja J. Armaković, Joseph Molnár, G. Spengler, V. Leovac, K. Meszaros Szecsényi
SYNTHESIS, STRUCTURAL AND THERMAL CHARACTERIZATION,
REACTIVITY ASSESSMENT BY DFT COMPUTATIONS AND BIOLOGICAL
EVALUATION OF A HYDRAZONE DERIVATIVE AND ITS COORDINATION
COMPOUNDS WITH CO(III), NI(II), CU(II) AND ZN(II)
New Journal of Chemistry 40 (2016) 5885-5895, (IF: 3.277)
17. **Stevan Armaković**, Sanja J. Armaković, Vladimir Holodkov, Svetlana Pelemiš
OPTOELECTRONIC PROPERTIES OF HIGHER ACENES, THEIR BN ANALOGUE
AND SUBSTITUTED DERIVATIVES
Materials Chemistry and Physics 170 (2016) 210-217, (IF: 2.259)
18. Milan Vraneš, Aleksandar Tot, **Stevan Armaković**, Sanja J. Armaković, Slobodan
Gadžurić
STRUCTURE MAKING PROPERTIES OF 1-(2-HYDROXYLETHYL)-3-
METHYLIMIDAZOLIUM CHLORIDE IONIC LIQUID
Journal of Chemical Thermodynamics 95 (2016) 174-179, (IF: 2.679)
19. Aleksandar Tot, **Stevan Armaković**, Sanja J. Armaković, Slobodan Gadžurić, Milan
Vraneš
KOSMOTROPISM OF NEWLY SYNTHESIZED 1-BUTYL-3-
METHYLIMIDAZOLIUM TAURATE IONIC LIQUID: EXPERIMENTAL AND
COMPUTATIONAL STUDY
Journal of Chemical Thermodynamics 94 (2016) 85-95 (IF: 2.679)
20. Milan Vraneš, **Stevan Armaković**, Aleksandar Tot, Snežana Papović, Nebojša Zec, Sanja
J. Armaković, Nemanja Banić, Biljana Abramović, Slobodan Gadžurić
STRUCTURING OF WATER IN THE NEW GENERATION IONIC LIQUID -
COMPARATIVE EXPERIMENTAL AND THEORETICAL STUDY
Journal of Chemical Thermodynamics 93 (2016) 164-171 (IF: 2.679)
21. **Stevan Armaković**, Sanja J. Armaković, Milan Vraneš, Aleksandar Tot, Slobodan
Gadžurić
DFT STUDY OF 1-BUTYL-3-METHYLIMIDAZOLIUM SALICYLATE: A THIRD-
GENERATION IONIC LIQUID
Journal of Molecular Modeling 21 (2015) 246-256 (IF: 1.867)
22. **Stevan Armaković**, Sanja J. Armaković, Jovan P. Šetrajčić, Vladimir Holodkov
AROMATICITY, RESPONSE, AND NONLINEAR OPTICAL PROPERTIES OF
SUMANENE MODIFIED WITH BORON AND NITROGEN ATOMS
Journal of Molecular Modeling 20 (2014) 2538-2551, (IF: 1.984)
23. **Stevan Armaković**, Sanja J. Armaković, Jovan P. Šetrajčić, Stevo K. Jaćimovski,
Vladimir Holodkov
SUMANENE AND ITS ADSORPTION PROPERTIES TOWARDS CO, CO₂ AND NH₃
MOLECULES
Journal of Molecular Modeling 20 (2014) 2170-2184, (IF: 1.984)
24. **Stevan Armaković**, Sanja J. Armaković, Jovan P. Šetrajčić, Ljubiša D. Džambas
SPECIFICITIES OF BORON DISUBSTITUTED SUMANENES
Journal of Molecular Modeling 19 (2013) 1153-1166, (IF: 1.984)

25. **Stevan Armaković**, Sanja J. Armaković, Jovan P. Šetrajčić, Igor J. Šetrajčić
ACTIVE COMPONENTS OF FREQUENTLY USED B-BLOCKERS FROM THE ASPECT OF COMPUTATIONAL STUDY
Journal of Molecular Modeling 18 (2012) 4491-4501, (IF: 1.984)
26. **Stevan Armaković**, Sanja J. Armaković, Svetlana Pelemiš, Jovan P. Šetrajčić
OPTOELECTRONIC AND CHARGE CARRIER HOPPING PROPERTIES OF ULTRATHIN BORON NITRIDE NANOTUBES
Superlattices and Microstructures 79 (2015) 79-85, (IF: 2.097)
27. **Stevan Armaković**, Sanja J. Armaković, Jovan P. Šetrajčić, Igor J. Šetrajčić
OPTICAL AND BOWL-TO-BOWL INVERSION PROPERTIES OF SUMANENE SUBSTITUTED ON ITS BENZYLIC POSITIONS; A DFT/TD-DFT STUDY
Chemical Physics Letters 578 (2013) 156-161, (IF: 2.337)
28. Jovan P. Šetrajčić, **Stevan Armaković**, Igor J. Šetrajčić, Ljubiša Džambas
SURFACE LOCALIZATION OF ELECTRONS IN ULTRATHIN CRYSTALLINE STRUCTURE
Modern Physics Letters B 28 (2014) 1450023-1450030, (IF: 0.746)

Citations

	Google Scholar	Scopus
Total number	141	90
h-index	7	5

Other

- Member of the Serbian Physical Society
- Member of the Materials Research Society of Serbia
- Member of Tendoryu Aikido club “Seiunkan” from Novi Sad
- Playing clarinet and guitar, basketball, writing
- Driver license, B category, active driver
- Married to Sanja with whom he has son Philip