CURRICULUM VITAE

Personal & Contact Information

Name: Julia Romanova
Address: Strelbishte, block 95, entrance A, flat 6, floor 3, 1404 Sofia, Bulgaria
E-mail: jromanova@chem.uni-sofia.bg, jromanova23@gmail.com
Nationality: Bulgarian
Date of Birth: 19.03.1983

Education

2007 – 2010 **Ph.D. in Chemistry**
University of Sofia (Bulgaria) & Université de Haute-Alsace (France)
Dissertation title: Influence of the medium on the geometry, electronic structure and magnetic properties of polyaniline (Theoretical and experimental investigation on structure, magnetic and conducting properties of conjugated N-containing oligomers)

2005 – 2006 **M.Sc. in Computational Chemistry**
University of Sofia, Bulgaria
Master thesis title: Theoretical investigation on the mechanism of Li - adsorption on pure and doped single-walled carbon nanotubes
GPA 5.86/6.00 and AG from thesis defense 6.00/6.00

2001 – 2005 **B. Sc. in Chemistry**
University of Sofia, Bulgaria
Profile: Physical Chemistry & Theoretical Chemistry
GPA 4.91/6.00 and AG from State Examinations 5.75/6.00

1996 – 2001 **High School Education**
High School for Science and Mathematics "Nancho Popovich", Shumen, Bulgaria

Research experience

2018 – **Assistant Professor**
University of Sofia, Faculty of Chemistry and Pharmacy, Department of Inorganic Chemistry, Bulgaria

2016 – 2018 **Maternity leave** (2 years)

2014 – 2016 **Research fellow** (2 years)
University of Surrey, Advanced Technology Institute, UK
Description: Computational Molecular Design of Type IV Metallopolymers and Stimuli-Responsive Organometallic complexes

2012 – 2014 **Postdoctoral researcher** (2.5 years)
University of Namur, Theoretical Chemistry Laboratory, Belgium
Description: Simulation of vibronic and resonance Raman spectra of viologens by DFT and multireference wavefunction methods (CASSCF/CASPT2)

2011 **Guest scientist** (3 months)
Leibniz Institute for Polymer Research Dresden, Theory of Polymers, Germany
Description: DFT investigations on the solvent effects in conducting polyaniline aiming to clarify its experimentally observed photovoltaic response

2011 **Postdoctoral researcher** (6 months)
University of Sofia, Bulgaria
Description: Theoretical investigation on the optical properties of conducting polyaniline as a function of its magnetic state: polaron and bipolaron form

Tutoring activity and teaching experience

2019 – **Teaching assistant**
University of Sofia, Bulgaria
Inorganic Chemistry - Laboratory exercises

2018 – **Tutoring students**
University of Sofia, Bulgaria

PhD students in the framework of a Scientific Projects (FNI-SU: № 80-10-22/22.03.2021):

- *Joanna Stoycheva*

Research students in the framework of a Scientific Projects (BSF: КП-06-Н39/2 from 09.12.2019; SF-SU: № 80-10-168/16.04.2019; SF-SU: № 80-10-3/18.03.2020):

- *Vaska Petakova* (Chemistry and Informatics, 2nd year Bachelor student)
- *Gergana Kostadinova* (Chemistry and Informatics, 2nd year Bachelor student)
- *Ilia Kichev* (Chemistry, 4th year Bachelor student)
- *Lyuben Borislavov* (Medicinal Chemistry, Master student)

Scientific consultant of Bachelor and PhD Thesis:

- *Joanna Stoycheva, "*Molecular modeling of components for energy conversion and energy storage devices", 1st year
- *Joanna Stoycheva, "*Molecular design of boron-doped anthracene and phenanthrene for singlet-fission-based photovoltaic materials*."* (supervisor Prof. Alia Tadjer)

- AQUACHIM award for the best Bachelor diploma in chemistry defended in 2018 in Bulgaria from: //www.aquachim.bg/uploads/media/stenik_catalogues/0001/01/153e660c80e93bf11b8f9e041167a79180170df0.pdf

2008 – 2009 **Teaching assistant**
University of Sofia, Bulgaria
Structure of Matter, Physical Chemistry and Molecular Design - Laboratory exercises

Awards

2018 **Best Poster Award**
"20th International Workshop on Nanoscience and Nanotechnology", Sofia, Bulgaria

2011 **'Eurika' Foundation Award for extraordinary achievements in science**

'Eurika' Foundation, Bulgaria
https://www.evrika.org/wp-content/uploads/2012/01/evrika-2011.pdf

Representative grants

2021 **PhD supporting Project**
Role: Principle investigator
Budget: 4700 BGN
Funding: *Science Fund – Sofia University*
Project number: № 80-10-22/22.03.2021
Project: Cumulenes – a key to the carbine structure mystery

2020 **Topical Project**
Role: Principle investigator
Budget: 3500 BGN
Funding: *Science Fund – Sofia University*
Project number: 80-10-3/18.03.2020
Principle Investigator: Julia Romanova
Project: Development of a prescreening model for the discovery of novel organic materials based on their diradical character

- Project SF-SU: № 80-10-3/18.03.2020 was selected as the best realized project from the Faculty of Chemistry and Pharmacy of the Sofia University for the financed year. https://www.uni-sofia.bg/index.php/bul/nauka/v_zmozhnosti_za_finansirane/programi/fond_nauchni_izsledvaniya_na_su

2019 – 2023 **Advanced Research Project**
Role: Principle investigator
Budget: 120 000 BGN
Funding: *Bulgarian Science Fund*
Project number: № КП-06-Н29/2 from 16.04.2019
Project: Machine learning for structure-properties relationship evaluation: the challenge in the hunt for singlet fission chromophores (https://ml4sf.chem.uni-sofia.bg/)

2019 **National L'Oréal-UNESCO fellowship for Women in Science**
Sofia, Bulgaria
https://www.zajenitevnaukata.bg/fellows2019.html

2019 **Topical Project**
Role: Principle investigator
Budget: 2500 BGN
Funding: *Science Fund – Sofia University*
Project number: FNI-SU: № 80-10-168/16.04.2019
Project: Boron doping and topology – new strategies for the design of organic photovoltaic materials

- Project SF-SU: № 80-10-168/16.04.2019 was selected as the best realized project from the Faculty of Chemistry and Pharmacy of the Sofia University for the financed year, https://www.uni-sofia.bg/index.php/bul/nauka/v_zmozhnosti_za_finansirane/programi/fond_nauchni_izsledvaniya_na_su/arhiv_konkursi/finansirane_ot_d_rzhavniya_byudzhet_konkurs_2020

2007 – 2010 **Mobility grant for international joint dissertation supervision** (3 years)
Role: Grant holder for PhD training
Funding: French Government
Project: Theoretical and experimental investigation on structure, magnetic and conducting properties of conjugated N-containing oligomers
Host Institutions: University of Sofia (Bulgaria) & Université de Haute-Alsace (France)

2006 **Short-term research grant for PhD students and young scientists** (3 months)
Role: Internship
Funding: German Academic Exchange Service (DAAD)
Project: Theoretical investigation on the structure-properties relationship in organic/inorganic hybrid spin molecular magnets
Host Institution: Max-Planck-Institute for Polymer Research (Germany)

- *2006 – 2021 Participation in more than 20 international and national research projects*

Scientific production

Publications more than 30 scientific papers in international journals with IF and peer-reviewed books; https://www.scopus.com/authid/detail.uri?authorId=36832298900

h-index 12

Patent 1; https://patents.google.com/patent/EP2268711A1/en

Selected talks presented at national and international conferences

2021 **High-throughput Extraction of Singlet Fission Chromophores for Photovoltaics Applications** (oral)
EUROPEAN CONGRESS AND EXHIBITION ON ADVANCED MATERIALS AND PROCESSES – EUROMAT, online, https://www.euromat2021.org/

2021 **Machine-learning-aided Discovery of Efficient Organic Photovoltaic Materials** (oral)
SizeMat 3: Third Workshop on Size-Dependent Effect in Materials for Environmental Protection and Energy Application, Pomorie, Bulgaria https://twinteam.igic.bas.bg/bg/sizemat/

2021 **Chasing Singlet Fission Chromophores for Organic Photovoltaics** (keynote lecture)
Virtual Conference on Chemistry and its Applications (VCCA), online, http://sites.uom.ac.mu/vcca2021/

2021 **Computational Screening for New Generation Photovoltaic Materials** (keynote lecture)
International Conference on Innovations in Energy Engineering & Cleaner Production IEECP, online, https://ieecp-conference.org/

2021 **Hunting for Singlet Fission Chromophores by Machine Learning Algorithms: the Diradical Character as a Preselection Rule** (oral)

CECAM Flagship Workshop "Materials Design for Energy Storage and Conversion: Theory and Experiment", online, https://www.cecam.org/workshop-details/25

2019 **Boron Doping as a Strategy for the Design of Efficient Organic Solar Cell Materials** (oral)
Tenth Jubilee National Conference on Chemistry, Sofia, Bulgaria, http://10ncc.unionchem.org/

2015 **The Role of Substituent Effects in Tuning Metallophilic Interactions and Emission Energy of bis-4-(2-Pyridyl)-1,2,3-triazolatoplatinum(II) Complexes** (invited lecture)
XXth International Workshop on Quantum Systems in Chemistry, Physics and Biology, Varna, Bulgaria, http://ntl.inrne.bas.bg/qscp2015/

2013 **Vibronic Coupling Effects in the Absorption and Resonance Raman Spectra of Extended Viologens** (oral)
XVIIIth Workshop on Theoretical Chemistry: Electron Correlation in Multireference Systems, Mini-symposium, Mariapfarr, Austria

2012 **New Insight into the Solvent and Dopant Effect on the Structure and Properties of Polyaniline** (oral)
Annual Meeting of the Belgian Polymer Group, Blankenberge, Belgium

- 2006-2021 Presentations in 24 national and international scientific conferences and workshops (12 posters and 12 oral presentations)

Computer skills

Electronic structure codes: *Gaussian, Molpro, Molcas, Gamess, Hyperchem, Mopac, Lumpac*
Programming: *Fortran, Unix shell scripting*

Languages

Bulgarian (native), English (very good), French (very good)

Academic service and contributions

Guest Editor of a Special Issue of Molecules-MDPI "Metal-Organic Complexes: Applications in Chemistry and Materials Science" 2020 (IF=4.411): https://www.mdpi.com/journal/molecules/special_issues/Organometallic

Reviewer: Journal of Organic Chemistry, Journal of Physical Chemistry, Journal of Computational Chemistry, Structural Chemistry, Photochemical & Photobiological Sciences, Open Chemistry, Journal of Molecular Liquids, Materialia, Applied Surface Science

Reviewer: ERC Frontier Research Grants

Scientific networks

Member of the L'Oréal-UNESCO For Women in Science Community:
https://community.forwomeninscience.com/addressbook/fullsearch/index?group_id=&isDegradedMode=false&degradedFilters=&from=0&size=24&q%5Ball%5D=romanova

ResearchGate: https://www.researchgate.net/profile/J-Romanova