Pavel Rukin

Modena Via Campi 213/A, 41125, Italy

Web of Science ResearcherID: AAA-3023-2019
ORCID: 0000-0002-9408-279

Personal information

Home Address:
Place and Date
Nationality: Russian Federation
Sex: Male
Marital status: Married
Current status: Ph.D in Physics and Mathematics, postdoctoral researcher, S3 Istituto Nanoscienze-CNR, Modena Via Campi 213/A, 41125, Italy.

Core competencies

- Ab Initio Electronic Structure Calculations
- Ab Initio-Based Normal Mode Analysis of Absorption/Emission Spectra
- Mixed Quantum Mechanical/Molecular Mechanical (QM/MM) Simulations
- Density Functional Theory (DFT), TDDFT

Educational Background

2021 online course "6.86x: Machine Learning with Python-From Linear Models to Deep Learning" of MITx (an online learning initiative of the Massachusetts Institute of Technology)

2018 Ph.D in Physics and Mathematics (Physical Chemistry), Lomonosov Moscow State University, Moscow, Russia

2011-2014 Ph.D student at the Photochemistry Center, Russian Academy of Sciences, Moscow, Russia

PhD Thesis Advisor: Prof. Alexander Bagaturyants, Ab Initio-Based Analysis of Vibronic Absorption Spectra of Dyes - Candidates for Chemosensor Applications

2011 Specialist (M.Sc.) in Applied Mathematics and Computer Science, National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), Moscow, Russia

M.Sc. Thesis Advisor: Prof. Alexander Bagaturyants, Modeling the Structures, Absorption and Emission Spectra of 9-Diphenylaminoacridine Dye Using DFT, DFT-D and TDDFT

Work Experience

2020-now postdoctoral researcher, S3 Istituto Nanoscienze-CNR, Via Campi 213/A, 41125, Modena, Italy.

2017-2020 junior research scientist, Federal Scientific Research Centre "Crystallography and Photonics" Photochemistry Center, Russian Academy of Sciences, ul. Novatorov 7a, Moscow, 119421 Russian Federation

2016-2017 Research engineer, Federal Scientific Research Centre "Crystallography and Photonics" Photochemistry Center, Russian Academy of Sciences, ul. Novatorov 7a, Moscow, 119421 Russian Federation

2015-2016 internship in University of Liège (Theoretical Physical Chemistry, UR MolSys B6c, University of Liège, B4000 Liège, Belgium)

2011-2015 Research engineer, Federal Scientific Research Centre "Crystallography and Photonics" Photochemistry Center, Russian Academy of Sciences, ul. Novatorov 7a, Moscow, 119421 Russian Federation

Research Experience

2020-now: Theoretical study of internal conversion between excited states in functionalized porphyrins. The tool of normal modes analysis for predicting design of the new organic components in case of functionalized porphyrins. S3 Istituto Nanoscienze-CNR (Advisors: Deborah Prezzi, Carlo Andrea Rozzi)

Rukin P., Prezzi D., Rozzi C.A. Excited-state normal-modes analysis: the case of porphyrins. J. Chem. Phys. 2023. DOI: 10.1063/5.0173336. (in press)

2016-2020: Molecular dynamics simulation of absorption and circular dichroism lineshapes of the rhodamine heterodimer tethered on DNA. The effect of environment and geometry distortion on the electronic properties of the chromophore is studied using QM/MD. Photochemistry Center, Russian Academy of Sciences (Advisor Prof. Alexander Bagaturyants) and University of Liège (Theoretical Physical Chemistry, UR MolSys B6c, University of Liège, B4000 Liège, Belgium, Advisor Prof. Françoise Remacle).

Rukin P.S., Komarova K.G., Fresch B., Collini E., and Remacle F. Chirality of arhodamine heterodimer linked to a DNA scaffold: an experimental and computationalstudy. Phys. Chem. Chem. Phys., 2020, 22,7516–7523.

Cipolloni M., Fresch B., Occhiuto I., **Rukin P.**, Komarova K.G., Cecconello A., Willner I., Levine R. D., Remacle F. Collini E., Phys. Chem. Chem. Phys. 2017, 19, 23043–23051. DOI: 10.1039/ C7CP01334E.

2013-2015: Vibronic bandshape of the absorption spectra of dibenzoylmethanatoboron difluoride

derivatives: an analysis based on ab initio calculations. Photochemistry Center, Russian Academy of Sciences (Advisor Prof. Alexander Bagaturyants). The nature of absorption bandshapes of dibenzoylmethanatoboron difluoride (DBMBF2) derivatives was theoretically investigated. Vibronic line broadening mechanism was analysed in terms of «soft» and «hard» vibrational modes.

P.S. Rukin, A.Ya. Freidzon, A.V. Scherbinin, V.A. Sazhnikov, A.A. Bagaturyants, M.V. Alfimov, Phys. Chem. Chem. Phys., 2015, 17, 26, 16997–17006. DOI: 10.1039/C5CP02085A.

2011-2013: Theoretical Study of the interaction of volatile amines with zinc porphyrins. Photochemistry Center, Russian Academy of Sciences (Advisor: Prof. Alexander Bagaturyants). The structures and absorption spectra of Zn(II) porphyrin (ZnP) and ZnTPP complexes with volatile amines were studied theoretically.

P.S. Rukin, P.A. Kashchenko, A.Yu. Malyavskaya, A.A. Bagaturyants, M.V. Alfimov, Nanotechnologies in Russia, 2014, 9, 3-4, 136-144 DOI: 10.1134/S199507801402013X

2010-2011: DFT calculations of fluorescent indicator 9-diphenylaminoacridine complexes with analytes. Photochemistry Center, Russian Academy of Sciences (Advisor Prof. Alexander Bagaturyants). The interaction between 9-diphenylaminoacridine (indicator) and several small analyte molecules was studied theoretically in view of the development of optical chemosensors based on organic dyes.

P.S. Rukin, A.A. Safonov, A.A. Bagaturyants, Nanotechnologies in Russia, 2011, Volume 6, Issue 5-6, 298-302. DOI 10.1134/S1995078011030141

Publication list

Papers:

1. **Rukin P.,** Prezzi D., Rozzi C.A. Excited-state normal-modes analysis: the case of porphyrins. J. Chem. Phys. 2023. DOI: 10.1063/5.0173336. (in press)
2. **Rukin P.S.,** Komarova K.G., Fresch B., Collini E., and Remacle F. Chirality of arhodamine heterodimer linked to a dna scaffold: an experimental and computational study. Phys. Chem. Chem. Phys., 2020, 22,7516–7523.
3. Cipolloni M., Fresch B., Occhiuto I., **Rukin P.**, Komarova K.G., Cecconello A., Willner I., Levine R.D., Remacle F., Collini E. Coherent electronic and nuclear dynamics in a rhodamine heterodimer–DNA supramolecular complex. Phys. Chem. Chem. Phys.,2017, 19, 23043–23051.
4. **Rukin P.S.**, Freidzon A.Y., Scherbinin A.V. et al.Vibronic bandshape of absorption spectra of dibenzoylmethanatoboron difluoride derivatives: Analysis based on ab initio calculations. Phys. Chem. Chem. Phys. 2015, 17, 26, 16997–17006.
5. **Rukin P.S.**, Kashchenko P.A., Malyavskaya A.Yu., Bagaturyants A.A., Alfimov M.V., Experimental and theoretical study of the interaction of volatile amines with zinc porphyrins. Nanotechnologies in Russia, 2014, 9, 3-4, 136–144.
6. **Rukin P.S.**, Safonov A.A., Bagaturyants A.A. Calculations of complexes of 9-diphenylamino-acridine fluorescent indicator with analyte molecules using density functional theory with dispersion correction. Nanotechnologies in Russia, 2011, 6, № 5-6, 298–302.

Conferences:

Contributed talks:

1. **Rukin P.S.,** Prezzi D., Rozzi C.A., "Theoretical Study Of Vibrational-Mediated Interlayer Charge Transfer In A Cobalt Phthalocyanine-Graphene Heterojunction. "Principles of light-induced charge transfer for optogenetics" CT4OPTO workshop. Modena. Italy. 3-5 July 2023.
2. **Rukin P.S.,** Petropoulos V., Quintela F., Russo M., Moretti L., Moore A., Moore T., Gust D., Prezzi D., Scholes G., Molinari E, Cerullo G., Troiani F., Rozzi C. A., Maiuri M. Exploring vibronically assisted ultrafast relaxation in a functionalized porphyrin with TDDFT and normal modes analysis. 9th Time-Dependent Density-Functional Theory: Prospects and Applications. Benasque. Spain. Oct 18 - Oct 28, 2022.
3. **Rukin P.S.,** Prezzi D., Rozzi C.A., "Theoretical study of internal conversion between B and Q bands in a functionalized porphyrin. "Principles of light-induced charge transfer for optogenetics" CT4OPTO workshop. 14-16 June 2021.Virtual.
4. **Rukin P.S.,** Komarova K.G., Fresch B., Cipolloni M., Remacle F. Environment Effects on the Optical Properties of a Rhodamine Heterodimer-DNA Supramolecular Complex: A computational and Experimental Study. Atomistic Simulation of Functional Materials (ASFM 2018). Moscow. Russia. 2018.
5. **Rukin P.S.,** Komarova K.G., Remacle F. Absorption lineshape analysis within nuclear-ensemble approximation of the rhodamine heterodimer based on molecular dynamics in complex media. «Atomistic Simulation of Functional Materials» (ASFM-2017 Winter). Moscow. Russia. 2017.
6. **Rukin P.S.,** Fresch B., Komarova K.G., Remacle F. Absorption spectrum analysis of the rhodamine-tamra dimer based on molecular dynamics in complex media. «Atomistic Simulation of Functional Materials» (ASFM-2016 Spring). Moscow. Russia. 2016. 22.
7. **Rukin P.S.,** Freidzon A.Ya, Scherbinin A.V., Bagaturyans A.A., Alfimov M.V. Theoretical study of absorption band shapes of dibenzoylmethanatoboron difluoride derivatives. «Atomistic Simulation of Functional Materials» (ASFM 2015-1). Moscow. Russia. 2015. 9.

Posters:

1. **Rukin P.S.,** Prezzi D., C.A. Rozzi, "Theoretical study of internal conversion between B and Q bands in a functionalized porphyrin. TYC IWOM 2021: International Workshop on Charge Transport and Excited State Processes in Organic Materials. 21-25 June 2021. Virtual. Poster.
2. **Rukin P.S.,** Fresch B., Komarova K.G., Remacle F. Absorption Spectrum Analysis of the Rhodamine-Tamra Dimer Based on Molecular Dynamics in Complex Media. Perspectives in Nano Information Processing an international conference and workshop. Cambridge. UK. 14-16 December. 2015.
3. **Rukin P.S.,** Freidzon A.Ya, Scherbinin A.V., Bagaturyans A.A., Alfimov M.V. Theoretical study of absorption band shapes of dibenzoylmethanatoboron difluoride derivatives. MPM (Modeling Photoactive Molecules). Nantes. France. 21-24 April. 2015. 64.
4. **Rukin P.S.,** Freidzon A.Ya, Scherbinin A.V., Bagaturyans A.A., Alfimov M.V. Theoretical study of absorption band shapes of dibenzoylmethanatoboron difluoride derivatives. European Materials Research Society (E-MRS) 2014 FALL MEETING, Warsaw University of Technology. Poland. 2014. K.K.8.

Awards

The Best Student Presentation In Symposium K (Computer modeling in nanoscience and nanotechnology: an atomic-scale perspective III). European Materials Research Society (E-MRS) 2014 FALL MEETING, Warsaw University of Technology, Poland, 2014.

References

Dr. Deborah Prezzi, CNR-Istituto Nanoscienze, Centro di Ricerca S3, Modena. (deborah.prezzi@nano.cnr.it)

Prof. Alexander Bagaturyants, Federal Scientific Research Centre "Crystallography and Photonics" Photochemistry Center, RAS (bagaturyants@gmail.com).

Prof. Françoise Remacle, Department of Chemistry, B6c, University of Liège (fremacle@ulg.ac.be)

Dr. Alexandra Freidzon, Federal Scientific Research Centre "Crystallography and Photonics" Photochemistry Center, RAS (freidzon.sanya@gmail.com).

Languages:

Russian (native), English (advanced), Italian (B1), French (A2).

Computer Skills

Programming: Python, Bash.

Quantum Chemistry and Molecular Dynamics packages:

Gamess-US, ORCA, Gaussian16, Amber, Gromacs, Newton-X.

Hobby

Dancing (Lindy Hop).