PAVEL RUBLEV

AFFILIATION

Department of Chemistry and Biochemistry, University of California, Los Angeles

EDUCATION

PhD University of California, Los Angeles, theory and computational chemistry, Los Angeles, California, USA — 2023-present

PhD Utah State University, Physical Chemistry, Logan, Utah, USA — 2021-2023
Incomplete

MS* Lomonosov Moscow State University, Physical Chemistry — 2015-2021
Graduated Summa Cum Laude

* Specialist degree corresponds to BS+MS degrees (6 years)

RESEARCH EXPERIENCE

University of California, Los Angeles, USA — 2023 to present.
Research Assistant, Advisor Name: Anastassia N. Alexandrova

- TBA

Utah State University, USA — 2021 to 2023
Research Assistant, Advisor Name: Alexander I. Boldyrev

- Molecular dynamics, Computational Spectroscopy
- Multiconfigurational electronic problems
- Conformational search problems, chemical bonding
- Property prediction for solid-body systems

Moscow State University, Russia — 2019 to 2021
Research Assistant, Advisor Name: Ilya O. Glebov

- Computational spectroscopy, excited states in biomolecules
- Property prediction for lanthanide complexes
- Multiconfigurational electronic problems

Moscow State University, Russia — 2015 to 2019
Research Assistant, Advisor Name: Valentina V. Utochnikova

- Experimental spectroscopy, luminescent materials
- Organic and inorganic synthesis

PUBLICATIONS

Journal Publications

10) Rublev, P.; Boldyrev, A.I., Scheiner, S. "Analysis of the Ability of C_6H_5I to Phosphoresce," *J. Phys. Chem. A*, 2023, 127, 23
DOI: 10.1021/acs.jpca.3c01678

9) Pozdeev A.S., Rublev P., Boldyrev A.I., "Bismuth Infrared Star: being at a glance," *Chemistry – A European Journal*, 2023
DOI: 10.1002/chem.202301663
*ASP and PR contributed equally

8) Pozdeev A.S., Rublev P., Boldyrev A.I., Rao Y., "Global Minimum Search and Bonding Analysis of Tl_2H_x and Tl_3H_y (x=0–6; y=0–5) Series," *ChemPhysChem*, 2023
DOI: 10.1002/cphc.202300332

7) Rublev, P., Tkachenko, N.V., Dub, P.A., and Boldyrev, A.I., "On the existence of CO_3^{2-} microsolvated clusters: a theoretical study," *Phys. Chem. Chem. Phys.*, 2023, 25
DOI: 10.1039/D3CP00955F

6) Pozdeev, A.S., Rublev, P., Boldyrev, A.I., Scheiner, S., "Theoretical Investigation of Geometries and Bonding of Indium Hydrides in the In_2H_x and In_3H_y (x = 0–4,6; y = 0–5) Series," *Molecules*, 2023, 28, DOI: 10.3390/molecules28010183

5) Rublev P., Tkachenko N.V., Pozdeev A.S., Boldyrev A.I., "Tinning the Carbon: Hydrostannanes Strike Back," *Dalton Trans.*, 2023, 52, DOI: 10.1039/D2DT03545F.
*NVT and PR contributed equally
(Highlighted as a Hot Article, featured on the Front Cover Page)

4) Rublev P., Tkachenko N.V., Boldyrev A.I., "Overlapping electron density and the global delocalization of π-aromatic fragments as the reason of conductivity of the biphenylene network," *J. Comput. Chem.,* 2023, 44, DOI: 10.1002/jcc.26854.

3) Tkachenko N.V., Rublev P., Dub P.A., "The Source of Proton in the Noyori–Ikariya Catalytic Cycle," *ACS Catal*., 2022, 12, DOI: 10.1021/acscatal.2c03540.
*NVT and PR contributed equally

2) Tkachenko N.V., Rublev P., Boldyrev A.I., Lehn J.M., "Superalkali Coated Rydberg Molecules," *Front. Chem.*, 2022, 10,880804, DOI: 10.3389/fchem.2022.880804.

1) Kovalenko A., Rublev P., Tcelykh L.O., Goloveshkin A.S., Lepnev L.S., Burlov A.S., Vashchenko A.A., Marciniak Ł., Magerramov A.M., Shikhaliyev N.G., Vatsadze S.Z., and Utochnikova V.V., "Lanthanide Complexes with 2-(Tosylamino)-benzylidene-N-

(aryloyl)hydrazones: Universal Luminescent Materials," *Chem. Mater.*, 2019, 31, 3, 759, DOI: 10.1021/acs.chemmater.8b03675

Journal Papers in Review

1) Melikyan G.G., Babayans N., Kalpakyan N., Herrera C., Rublev P., Tkachenko N.V., Boldyrev A.I., "Cobalt-complexed acetylenic tetrads, a novel molecular scaffold for quadruple ionic functionalization reactions.," submitted to: *Journal of American Chemical Society*

PRESENTATIONS AND INVITED LECTURES

1. *International Conference on Chemical Bonding*, Invited Talk, "Revealing of $NdCl_3$ speciation in aqueous solutions by QM/MM molecular dynamics simulations"
   ‖ 11-17 August 2022, Kauai, USA.

2. *Goldschmidt2022*, "Evaluation of aqueous speciation of Nd a in chloride-bearing solutions by QM/MM dynamics"
   ‖ 10-16 July 2022, O'ahu, USA.

3. *MSU-IFW-ILTPE Joint Workshop. Synthesis, Theoretical Examination and Experimental Investigation of Emergent Materials*, "Synthesis and Luminescent Properties Of Lanthanide Complexes With Substituted 2-Tosylaminobenzoylhydrazones"
   ‖ 2-7 October 2017, Nizhny Novgorod, Russia.

4. *27th International Chugaev Conference on Coordination Chemistry*, "Approaches to improve lanthanide NIR luminescent features"
   ‖ 14-16 June 2017, Moscow, Russia.

TEACHING EXPERIENCE

1. *Teaching Assistant:* Organic Chemistry II (CHEM 2320), Spring 2023

2. *Teaching Assistant:* General Chemistry II Laboratory (CHEM 1125), Spring 2022

INTERNSHIPS

Schrodinger, Inc.
Summer intern — Summer 2023

Project: Realistic simulation of chemical reactivity
with Born-Oppenheimer Molecular Dynamics

Los Alamos National Laboratory
Graduate research assistant Summer 2022
Project: Molecular complexation of rare earth elements (REE)
in high temperature and pressure

LANGUAGES

Russian: Native Language

English: Advanced

SKILLS IN COMPUTATIONAL CHEMISTRY

Molecular problems: GAMESS US, Firefly (formerly PC GAMESS), ORCA, QChem, Jaguar, OpenMolcas, Gaussian, xTB\CREST

"Bulk" problems with PBC: CP2K, VASP, Quantum Espresso, Abinit, DFTB+

Classical molecular dynamics: AMBER, Desmond