Adil Kabylda

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Education

2021–202x **(Expected) Ph.D. in Physics and Materials Science**, University of Luxembourg

2015–2021 **B.Sc. and M.Sc. in Fundamental and Applied Chemistry (summa cum laude)**, *Lomonosov Moscow State University*, GPA: 3.93/4.00

Professional Experience

2021–Present **Theoretical Chemical Physics Group**, *University of Luxembourg*
Project: Development of accurate machine learning models for large and flexible molecules.
Advisor: Professor Alexandre Tkatchenko – alexandre.tkatchenko@uni.lu

2022 **Institute for Pure and Applied Mathematics**, *UCLA, Los Angeles*
Visiting Researcher at "Advancing Quantum Mechanics with Mathematics and Statistics" Long Program.

2018–2021 **Laboratory of Quantum Photodynamics**, *Lomonosov Moscow State University*
Project I: Studied the nature of light-induced phenomena of the GFP chromophore and its chemically modified versions using state-of-the-art quantum chemistry methods.
Project II: Investigated the molecular mechanism of retinal thermal isomerization and kinetics of retinal chromophore fragmentation.
Advisor: Associate Professor Anastasia Bochenkova – bochenkova@phys.chem.msu.ru

2018 **TCH Laboratory**, *Nanyang Technological University*, Singapore
Project: Synthesized new bisguanidinium-type phase-transfer catalyst. Performed comparative analysis of experimental/calculated Infrared and Raman data.
Advisor: Professor Tan Choon-Hong – choonhong@ntu.edu.sg

2017 **Laboratory of Laser Diagnostics**, *Lomonosov Moscow State University*
Project: Conducted research on the selection of a suitable molecular form of chlorine in the plasma and its determination in concrete by the LIBS method.
Advisor: Associate Professor Timur Labutin – timurla@laser.chem.msu

2015–2018 **Laboratory of Organic Synthesis**, *Lomonosov Moscow State University*
Project I: Developed an efficient way for the synthesis of peptide fragment of natural depsipeptides Jaspamide and Chondramide by means of Ugi reaction.
Project II: Studied multicomponent azido-Ugi reaction of natural alkaloid cytisine.
Advisor: Professor Valentine Nenajdenko – nenajdenko@org.chem.msu.ru

Publications (* - indicates equal contribution)

1. **A. Kabylda***, V. Vassilev-Galindo*, S. Chmiela, I. Poltavsky, A. Tkatchenko. Efficient Interatomic Descriptors for Accurate Machine Learning Force Fields of Extended Molecules. Nat. Commun. **2023**, accepted.
2. S. Chmiela, V. Vassilev-Galindo, O.T. Unke, **A. Kabylda**, H.E. Sauceda, A. Tkatchenko, K.-R. Muller. Accurate Global Machine Learning Force Fields for Molecules with Hundreds of Atoms. Sci. Adv. **2023**, 9, 2, eadf0873.
3. E. Gruber*, **A.M. Kabylda***, M.B. Nielsen, A.P. Rasmussen, R. Teiwes, P.A. Kusochek, A.V. Bochenkova, L.H. Andersen. Light Driven Ultrafast Bioinspired Molecular Motors: Steering and Accelerating Photoisomerization Dynamics of Retinal. J. Am. Chem. Soc. **2022**, 144, 1, 69–73.
4. J. Langeland, N.W. Persen, E. Gruber, H.V. Kiefer, **A.M. Kabylda** †, A.V. Bochenkova, L.H. Andersen. Controlling light-induced proton transfer from the GFP chromophore. *ChemPhysChem* **2021**, 22 (9), 807-807. *first theory author*†. ***Selected as cover article.***
5. D.A. Gorbachev*, E.F. Petrusevich*, **A.M. Kabylda***, E.G. Maksimov, K.A. Lukyanov, A.M. Bogdanov, M.S. Baranov, A.V. Bochenkova, A.S. Mishin. A General Mechanism of Green-to-Red Photoconversions of GFP. *Front. Mol. Biosci.* **2020**, 7, 176.
6. K.F. Chin, X. Ye, Y. Li, R. Lee, **A.M. Kabylda**, D. Leow, X. Zhang, E.C.X. Ang, C.-H. Tan. Bisguanidinium-Catalyzed Epoxidation of Allylic and Homoallylic Amines under Phase Transfer Conditions. *ACS Catal.*, **2020**, 10, 4, 2684–2691. ***Selected as cover article.***
7. D.P. Zarezin, O.I. Shmatova, **A.M. Kabylda**, and V.G. Nenajdenko. Efficient synthesis of the peptide fragment of the natural depsipeptides Jaspamide and Chondramide. *Eur. J. Org. Chem.*, **2018**, 2018 (34), 4716–4722.

8. D.P. Zarezin, **A.M. Kabylda**, V.I. Vinogradova, P.V. Dorovatovskii, V.N. Khrustalev, and V.G. Nenajdenko. Efficient synthesis of tetrazole derivatives of cytisine using the azido-Ugi reaction. *Tetrahedron*, **2018**, 74 (32), 4315-4322.

Conference Talks

1. ESTML 2023. *Machine Learning Force Fields for Large Molecules.* Levi, Finland, April **2023**.
2. TSRC workshop on "Intermolecular Interactions: New Challenges for *ab initio* Theory". *Understanding Interatomic Interactions in Large Molecules from Machine-Learned Force Fields.* Telluride, Colorado, March **2023**.
3. ACS Fall Meeting. *Optimizing Descriptors for Accurate Machine Learning Force Fields of Large Molecules.* online, August **2022**.
4. IPAM "Advancing Quantum Mechanics with Mathematics and Statistics" Long Program. *Interatomic Features for Accurate Machine Learning Force Fields of Large Molecules.* Los Angeles, May **2022**.
5. DQML conference 2022. *Optimizing Descriptors for Accurate ML Modeling of Large and Flexible Molecules.* Hintertux, Austria, February **2022**.
6. Lomonosov 2021. *Effect of chemical modifications on the mechanism and kinetics of retinal photoisomerization.* **Best Oral Presentation**. Moscow, April **2021**.
7. CECAM Workshop, Virtual Winter School on Computational Chemistry. *Thermal isomerization of the retinal in the gas phase: a detailed XMCQDPT2 study.* online, February **2021**.
8. Lomonosov 2020. *Molecular mechanism of the retinal chromophore thermal isomerization.* **Best Oral Presentation**. Moscow, November **2020**.

Awards and Honors

2022 Alumni of the 71st Lindau Nobel Laureate Meeting dedicated to Chemistry with 30 Nobel Laureates: selected in a world wide competition between young scientists

2021 FNR AFR Individual PhD Fellowship

2021 Graduated Summa Cum Laude

2021 Best thesis work in Physical Chemistry

2018 – 2021 Increased State Academic Scholarship: Awarded by the MSU Chemistry Department for outstanding scientific achievements

2020 Silver medal at the Yandex "I'm professional" olympiad, Physical Chemistry and Catalysis

2016 Student of the year: awarded by the MSU rector for outstanding achievements to 5 students across all departments

2015 Valedictorian of Pavlodar Region, Kazakhstan

2015 Gold medal at the 47th International Chemistry Olympiad in Baku, Azerbaijan

2014 Silver medal at the 46th International Chemistry Olympiad in Hanoi, Vietnam

Teaching and Service

2023 Co-organizer of ESTML 2023 Workshop in Levi, Finland

2022 Teaching assistant in Quantum Mechanics course, University of Luxembourg

2021 Teaching assistant in Advanced Physical Chemistry course, MSU

2020 – 2021 Co-supervised 3 undergraduate students' semester projects in Physical and Quantum Chemistry

2019 Member of Team Moscow at iGEM 2019: supervised and guided a student in the kinetic modeling of biomolecular interactions

2015 – 2021 Lecturer in Physical and Quantum Chemistry for Kazakhstan national/regional high-school chemistry team

2015 – 2016 Jury at Regional Chemistry Olympiad, Pavlodar, Kazakhstan

2015 Author in OYLA popular-scientific magazine, Almaty, Kazakhstan