Martin Vondrák

Date of Birth: 29. 7. 1996

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Current research interest

- Machine learning electrostatic interactions in materials

Past Research interests

- Molecular mechanics simulations of graphene
- Interactions of small RNA hairpins with graphene
- Molecular dynamics simulations of graphene based supercapacitors

Work Experience

2021–now	**Ph.D. candidate position at the Fritz Haber Institut MPG and the University of Bayreuth, Germany**
2015–2021	Science center Fort Science I worked as an edutainer in math, physics and chemistry exhibitions.

Education

2024–now	Ph.D. candidate at the University of Bayreuth, Germany. Supervised by Dr. Johannes Margraf, and Prof. Karsten Reuter
10.-12. 2023	Visiting student in the group of Professor Gábor Csányi, Department of Engineering Engineering of Cambridge University, Cambridge, United Kingdom
2021–2023	Ph.D. candidate at the Fritz Haber Institut MPG, Germany. Supervised by Dr. Johannes Margraf, and Prof. Karsten Reuter
2019–2021	MSc in Physical Chemistry, Palacký University, Czech Republic Final exams with marks (the scale of grades from A (best) to F (worst)): Modeling of biostructures and bioinformatics (**A**), Quantum Chemistry and Chemical Structure (**A**), Analytical Chemistry (**A**), Physical Chemistry (**A**), Final MSc Thesis Defense (**A**)
2019–2021	Qualification Course for Teachers of Chemistry, Palacký University, CR
2016–2019	BSc in Chemistry, Palacký University, Czech Republic Final exams with marks (the scale of grades from A (best) to F (worst)): General and Inorganic Chemistry (**A**), Organic Chemistry (**A**), Analytical Chemistry (**B**), Physical Chemistry (**A**), Final BC Thesis Defense (**A**)

Publications and Awards

2023 First author of Vondrák, M. et al. q-pac: A Python package for machine learned charge equilibration models. J. Chem. Phys. 159, 054109 (2023)

2022 Author of Pykal, M. et al. Accessibility of Grafted Functional Groups Limits Reactivity of Covalent Graphene Derivatives. Appl. Surf. Sci. 598, (2022)

2018 Coauthor of Li, Q. et al. RNA nanopatterning on graphene. 2D Mater. 5, (2018)

2016 Students' Professional Activities, 3rd place in Chemistry category
Name of the project: Structural Changes Accompanying the Process of Graphene Oxidation

2015 Czech Little Head Genus 2015 Award

2015 The Learned Society Award for Students' Professional Activities

2015 Students' Professional Activities, 2nd shared (50 %) place in Chemistry category
Name of the project: The Catalysis of the Nucleolytic Ribozymes

2015 Students' Professional Activities, 4th place in Math category
Name of the project: Statistical Analysis of Composition Tables in Coordinates

2014 Students' Professional Activities, 5th place in Math category
Name of the project: Statistic Analysis of Independence in Four-field Data Tables

Other Activities

2019 Foundation of Reproducibilitea in Olomouc, Czech Republic
Czech branch of global journal club started 2016 at University of Oxford initiative focused on open and reproducible science, founded and organized by Chemistry Club UP

2017 Foundation of Chemistry club UP
Student organization at Palacký University holding lectures from chemistry given by experts, popularizing chemistry for high school students and organizing excursions in chemistry laboratories

2016 Participation on the international conference MILSET Expo-Sciences Europe 2016
Presentation of the project The Catalysis of the Nucleolytic Ribozymes at the MILSET Expo-Sciences Europe 2016 in Toulouse, France

2015 World Science Conference – Israel
Workshops and lectures from Nobel laureates, research-based Israeli companies, and researchers from Hebrew University of Jerusalem.