

Marius Kadek

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Current position

2018–present **Researcher**, *Faculty of Science and Technology, UiT – The Arctic University of Norway, Tromsø, Norway.*

Education

2014–2018 **Doctor of Philosophy (PhD)**, *Faculty of Science and Technology, UiT – The Arctic University of Norway, Tromsø, Norway.*

2011–2013 **Master of Science**, *Faculty of Mathematics, Physics and Informatics, Comenius University, Bratislava, Slovakia.*
theoretical physics study program

2008–2011 **Bachelor's degree**, *Faculty of Mathematics, Physics and Informatics, Comenius University, Bratislava, Slovakia.*
physics study program

Dissertation thesis

title *Advancing relativistic electronic structure methods for solids and in the time domain*
supervisor Kenneth Ruud, Institute of Chemistry, UiT, Tromsø
co-supervisor Michal Repisky, Institute of Chemistry, UiT, Tromsø
description Solving the 4-component Dirac–Kohn–Sham equation for periodic systems using Gaussian-type one-particle basis functions.

Master thesis

title *Analysis of electron excitation in molecules using a real-time time-dependent Dirac–Coulomb method*
supervisor Vladimir Malkin, Institute of Inorganic Chemistry, Slovak Academy of Sciences, Bratislava

Bachelor thesis

title *Homogeneous and isotropic tensors*
supervisor Marian Fecko, Department of Theoretical Physics, Comenius University, Bratislava

Teaching

2016–2017 **teaching assistant**, *Department of Physics and Technology, UiT – The Arctic University of Norway, Tromsø.*
FYS-2000 Quantum mechanics

Fall 2014 **teaching assistant**, *Department of Physics and Technology, UiT – The Arctic University of Norway, Tromsø.*
FYS-2001 Statistical physics and thermodynamics

Fall 2013 **teaching assistant**, *Department of Theoretical Physics, Comenius University, Bratislava.*
1-FYZ-251/15 Theoretical mechanics

International schools

- 13.–19.3.2016 **Molecular Response Properties Winter School**, Superbagnères de Luchon, France.
6.–19.9.2015 **15th European Summer School in Quantum Chemistry**, Sicily, Italy.
1.–13.7.2012 **12th Sostrup Summer School**, Himmelbjerget, Denmark.

Selected conferences

- 3.–7.9.2018 **Flatlands Beyond Graphene 2018**, Leipzig, Germany.
2.–6.9.2017 **REHE 2017**, 12th International Conference on Relativistic Effects in Heavy-Element Chemistry and Physics, Marburg, Germany.
27.8.–1.9.2017 **WATOC 2017**, 11th Triennial Congress of the World Association of Theoretical and Computational Chemists, Munich, Germany.
22.–23.4.2015 **CTCC annual meeting**, Sundvolden, Norway.
Oral presentation: "A solution of the TDDFT equation in real time".
22.–27.2.2015 **Workshop on Modern Methods in Quantum Chemistry**, Mariapfarr, Austria.
Oral presentation: "4-component real-time TDDFT (theory and implementation)".
20.–24.9.2014 **REHE 2014**, 11th International Conference on Relativistic Effects in Heavy-Element Chemistry and Physics, Smolenice, Slovakia.
Poster presentation: "Real-time solution of the time-dependent Dirac-Coulomb equation".

Publications

5. [M. Kadek](#), M. Repisky, K. Ruud: All-electron fully relativistic Kohn-Sham theory for solids based on the Dirac-Coulomb Hamiltonian and Gaussian-type functions, *Phys. Rev. B*, **99**, 20, 205103, (2019) DOI: [10.1103/PhysRevB.99.205103](https://doi.org/10.1103/PhysRevB.99.205103)
4. L. Konecny, [M. Kadek](#), S. Komorovsky, K. Ruud, M. Repisky: Resolution-of-identity accelerated relativistic two- and four-component electron dynamics approach to chiroptical spectroscopies, *J. Chem. Phys.*, **149**, 20, 204104, (2018) DOI: [10.1063/1.5051032](https://doi.org/10.1063/1.5051032)
3. L. Konecny, [M. Kadek](#), S. Komorovsky, O. L. Malkina, K. Ruud, M. Repisky: Acceleration of Relativistic Electron Dynamics by Means of X2C Transformation: Application to the Calculation of Nonlinear Optical Properties, *J. Chem. Theory Comput.*, **12**, 12, 5823-5833, (2016) DOI: [10.1021/acs.jctc.6b00740](https://doi.org/10.1021/acs.jctc.6b00740)
2. [M. Kadek](#), L. Konecny, B. Gao, K. Ruud: X-ray absorption resonances near $L_{2,3}$ -edges from real-time propagation of the Dirac-Kohn-Sham density matrix, *Phys. Chem. Chem. Phys.* **17**, 22566–22570 (2015) DOI: [10.1039/c5cp03712c](https://doi.org/10.1039/c5cp03712c)
1. M. Repisky, L. Konecny, [M. Kadek](#), S. Komorovsky, O. L. Malkin, V. G. Malkin, K. Ruud: Excitation Energies from Real-Time Propagation of the Four-Component Dirac-Kohn-Sham Equation, *J. Chem. Theory Comput.*, **11**, 3, 980-991, (2015) DOI: [10.1021/ct501078d](https://doi.org/10.1021/ct501078d)

Awards

- June 2013 **award from the rector of Comenius University**.
for outstanding fulfillment of study duties throughout the entire time at university
- May 2012 **"Young Head" award of Slovenský plynárenský priemysel (Slovak Gas Industry)**.
scholarship to co-finance the attendance of the 12th Sostrup Summer School
- May 2012 **Tatra banka scholarship "Students to the World"**.
scholarship to co-finance the attendance of the 12th Sostrup Summer School

April 2008 **2nd place on the national round of High School Technical Competition in category “Mathematics, Physics”.**
high school science fair

Other experience

2011–present **Developer of ReSpect quantum-chemical software.**
homepage: <http://respectprogram.org/mariuskadek.html>

18.–24.4.2017 **Research stay**, *Central European Institute of Technology*, Brno, Check Republic.

2011–2013 **Organizer of “Trojsten” Physics Correspondence Seminar**, Bratislava.
organizing physical correspondence competition for high school students, giving popular lectures

Skills

programming Fortran, Python, Haskell, Java
technical Mathematica, Git, LaTeX
language English