

Lukáš Konečný

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Current position

04/2018– **Postdoc**, *Hylleraas Centre for Quantum Molecular Sciences, UiT The Arctic University of Norway*, Tromsø, Norway.

Publications

M. Repisky, S. Komorovsky, M. Kadek, L. Konecny, U. Ekstrom, E. Malkin, M. Kaupp, K. Ruud, O. L. Malkina, V. G. Malkin: ReSpect: Relativistic Spectroscopy DFT program package, *accepted for publication in J. Chem. Phys*

L. Konecny, M. Repisky, K. Ruud, and S. Komorovsky: Relativistic four-component linear damped response TDDFT for electronic absorption and circular dichroism calculations *J. Chem. Phys.* **151**, 194112 (2019), DOI: [10.1063/1.5128564](https://doi.org/10.1063/1.5128564)

L. Konecny, M. Kadek, S. Komorovsky, K. Ruud, and M. Repisky: Resolution-of-identity accelerated relativistic two- and four-component electron dynamics approach to chiroptical spectroscopies *J. Chem. Phys.* **149**, 204104 (2018) DOI: [10.1063/1.5051032](https://doi.org/10.1063/1.5051032)

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)

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)

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)

Education

2013–2017 **Doctoral degree**, *Faculty of Natural Sciences, Comenius University*, Bratislava, Slovakia.
Chemical Physics

2011–2013 **Master degree**, *Faculty of Mathematics, Physics and Informatics, Comenius University*, Bratislava, Slovakia.
Theoretical Physics

2008–2011 **Bachelor degree**, *Faculty of Natural Sciences, Comenius University*, Bratislava, Slovakia.
Chemistry

Dissertation

title *Development of advanced methods for the relativistic calculations of electronic structure*
supervisor Oľga Malkin, Institute of Inorganic Chemistry, Slovak Academy of Sciences, Bratislava

description Implemented electron dynamics (real-time TDDFT) and linear response theory solution of the time-dependent Dirac equation based on the four-component Dirac–Coulomb and the two-component X2C Hamiltonian; and developed analysis tools to interpret simulation results.

Experience

Scientific

- 11/15–5/16 **Research stay**, *The Centre for Theoretical and Computational Chemistry*, Tromsø, Norway.
1–2/2015 **Research stay**, *The Centre for Theoretical and Computational Chemistry*, Tromsø, Norway.
2011– **Developer of quantum-chemical software**.
Computer program ReSpect (homepage: <http://www.respectprogram.org/>).

Pedagogical

- 09/2017– **Lecturer**, *Faculty of Natural Sciences, Comenius University*, Bratislava.
04/2018 Chemical Calculations.
2013–2017 **Teaching Assistant**, *Faculty of Natural Sciences, Comenius University*, Bratislava.
Seminars for General Chemistry classes.

Conferences

- 8–9/10/19 **NKS 2019**, Meeting of the Quantum and Computational Chemistry Section of the Norwegian Chemical Society, Trondheim, Norway.
Invited talk.
- 11–17/8/19 **ISTCP 2019**, 10th Triennial Congress of the International Society for Theoretical Chemical Physics, Tromsø, Norway.
Poster presentation.
- 4–8/3/19 **APS March Meeting 2019**, Boston, Massachusetts, USA.
Oral presentation.
- 16–18/10/18 **NKS 2018**, 21st Meeting of the Norwegian Chemical Society, Lillestrøm, Norway.
Oral presentation.
- 9–12/9/18 **CESTC 2018**, 16th Central European Symposium on Theoretical Chemistry, Srní, Czech Republic.
Poster presentation.
- 18–23/6/18 **ICQC 2018**, 16th International Congress on Quantum Chemistry, Menton, France.
Poster presentation.
- 8–9/1/18 **Our Astro-Chemical History**, COST action 1401 WG3 workshop Formation and destruction of molecules by UV and X-ray radiation, Bristol, UK.
Oral presentation.
- 2–6/9/17 **REHE 2017**, 12th International Conference on Relativistic Effects in Heavy-Element Chemistry and Physics, Marburg, Germany.
Poster presentation.
- 27/8–1/9/17 **WATOC 2017**, 11th Triennial Congress of the World Association of Theoretical and Computational Chemists, Munich, Germany.
Poster presentation.
- 19–24/2/17 **Sanibel Symposium**, St. Simons Island, Georgia, USA.
Poster presentation.

- 5–7/4/16 **CTCC Spring Meeting**, Meeting of the Centre for Theoretical and Computational Chemistry, Alta, Norway.
Oral presentation.
- 23–28/2/16 **Workshop on Modern Methods in Quantum Chemistry**, Mariapfarr, Austria.
Oral presentation.
- 11–14/10/15 **JCS 2015**, 6th Japan–Czech–Slovak Symposium on Theoretical Chemistry, Smolenice, Slovakia.
Poster presentation.
- 22–27/2/15 **Workshop on Modern Methods in Quantum Chemistry**, Mariapfarr, Austria.
Oral presentation.
- 20–25/9/14 **REHE 2014**, 11th International Conference on Relativistic Effects in Heavy-Element Chemistry and Physics, Smolenice, Slovakia.
Poster presentation.

Schools

- 13–19/3/2016 **Molecular Response Properties Winter School**, Superbagnères de Luchon, France.
- 6–19/9/2015 **15th European Summerschool in Quantum Chemistry**, Hotel Torre Normanna, Italy.
- 25/8–5/9/2014 **5th Summer School on Modern Computational Science (MCS)**, Oldenburg, Germany.
Topic: computational quantum chemistry.
- 1–13/7/12 **12th Sostrup Summer School**, Ry, Denmark.
Topic: quantum chemistry and molecular properties.

Awards

- 2016 **Comenius University grant for young researchers.**
- 2015 **National Scholarship Programme of the Slovak Republic (NSP).**
Travel grant for the research stay in Tromsø, Norway
- 2015 **Comenius University grant for young researchers.**
- 2014 **DAAD grant to cover the attendance of MCS Summer School 2014.**
- 2012 **“Young Head” award of Slovenský plynárenský priemysel (Slovak gas industry).**
Scholarship to co-finance the attendance of the 12th Sostrup Summer School
- 2012 **Tatra banka scholarship “Students to the World”.**
Scholarship to co-finance the attendance of the 12th Sostrup Summer School

Past achievements

- 12–21/7/2008 **International Chemistry Olympiad**, Budapest, Hungary, bronze medal.
- 25/3–1/4/2007 **European Union Science Olympiad**, Potsdam, Germany, silver medal.
- 2–8/4/2006 **European Union Science Olympiad**, Brussels, Belgium, silver medal.