MICHAL REPISKY

Faculty of Natural Sciences
Comenius University

Project number
3129/01/02

Project duration
7/2022 - 9/2025

"The SASPRO2 fellowship represents for me a unique opportunity to pursue individual research activities in the field of molecular and material properties driven by spin–orbit interaction, aiding thus experimental community to design novel and unique materials. The teaching and supervision responsibilities also enable me to bring the research front in relativistic modelling to undergraduate and graduate students."

BIOGRAPHY

Michal Repisky received his Ph.D. degree from the Slovak Academy of Sciences in 2009 and spent 3 years as a postdoctoral fellow in Tromsø (Norway) with Prof. Kenneth Ruud, before starting his professional career as a junior researcher at the Department of Chemistry, University of Tromsø. From 2022, he holds the principal investigator position at the Hylleraas Centre for Quantum Molecular Sciences, Norwegian Centre of Excellence.

Michal Repisky's main research interests are development and application of modern relativistic ab-initio electronic structure methods based on the multicomponent Pauli and Dirac formalism for the study of molecular and material properties, with a particular focus on magnetic resonance phenomena. Additional interests include response theory for molecules and solids, real-time electron dynamics, and high-performance computing. He is also the team leader behind the development of relativistic quantum chemistry DFT program, ReSpect (*www.respectprogram.org*).

PROJECT SUMMARY

EPR and NMR Spectroscopy of Spin–Orbit-Coupled Paramagnetic Solids

Unpaired electrons play a key role in many chemical and physical processes, such as electron transport in lithium or sodium transition metal oxide-based battery materials or at catalytically active sites in metal-organic frameworks (MOFs). In order to optimise the performance of such materials, the relation between the structure and properties of materials must be established. Electron paramagnetic resonance (EPR) and paramagnetic nuclear magnetic resonance (pNMR) spectroscopy allow the structure of paramagnetic materials to be established, often aided and supported by computational studies that can help relate experimental spectra to details in the electronic structure of materials, and in this way facilitate the design of more efficient materials. However, whereas the theoretical calculation of EPR and NMR spectra are well established for molecules in gas and liquid phases, and non-relativistic approaches for NMR spectra of closed-shell molecules exists for solids, there is currently no relativistic approach for the calculation of NMR spectra of paramagnetic solids, leaving a major gap in the ability of computational chemistry/physics to contribute to rationalising structure-property relationships of such solid-state materials. This project will fill this gap by developing an all-electron two- and four-component relativistic density-functional theory modeling framework for the calculation of EPR and paramagnetic NMR spectra of solids. The project will build on our recently developed four-component DFT code for solids and our recent advances in relativistic calculations of EPR and pNMR spectra of molecules to make a major step forward in the modeling of magnetic solids. This will allow us to advance the use of EPR and pNMR to the study of paramagnetic solids, and the inclusion of relativistic effects will allows us to reliably describe paramagnetic solids with heavy elements, such as lithium or sodium transition metal oxides, of relevance as battery materials.

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PUBLICATIONS

1. Knecht et al., *Exact two-component Hamiltonians for relativistic quantum chemistry: Two-electron picture-change corrections made simple*, Journal of Chemical Physics, just accepted (2022).

2. Konecny et al., *Accurate X-ray Absorption Spectra near L- and M-Edges from Relativistic Four-Component Damped Response Time-Dependent Density Functional Theory,* Inorganic Chemistry 61, 830-846 (2022).

3. Pototschnig at al., *Implementation of Relativistic Coupled Cluster Theory for Massively Parallel GPU-Accelerated Computing Architectures*, Journal of Chemical Theory and Computation 17, 5509-5529 (2021).

4. Senjean at al., *Generalization of intrinsic orbitals to Kramers-paired quaternion spinors, molecular fragments and valence virtual spinors,* Journal of Chemical Theory and Computation 17, 1337-1354 (2021).

5. Repisky at al., *ReSpect: Relativistic spectroscopy DFT program package*, Journal of Chemical Physics 152, 184101 (2020).

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This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No. 945478.