

# Curriculum Vitae

Zilvinas Rinkevicius  
Department of Theoretical Chemistry  
School of Biotechnology  
KTH, S-106 91 Stockholm, Sweden

## Personal information

**Name:** Zilvinas Rinkevicius

**Date of Birth:** 1978 January 21, Prienai, Lithuania

**Work address, phone, e-mail:**

Department of Theoretical Chemistry  
School of Biotechnology  
KTH, S-106 91 Stockholm, Sweden

*Phone:* +46 (0)8 5537 8416

*Fax:* +46 (0)8 5537 8590

*E-mail:* rinkevic@theochem.kth.se

**Present employment:**

Lector (Lektor) at Department of Theoretical Chemistry, School of Biotechnology, KTH (date of appointment 2010-07-01), supported by Swedish E-science Center (SerC), KTH

**Previous employments:**

*2008-05-01-2010-06-30:* Researcher (Forskare) at Department of Theoretical Chemistry, School of Biotechnology, KTH.

*2007-05-01-2008-04-30:* Researcher (Forskare) at Department of Theoretical Chemistry, School of Biotechnology, KTH.

*2005-05-01-2007-04-30:* Research assistant (Forskarassistent) at Department of Theoretical Chemistry, School of Biotechnology, KTH.

*2004-06-01-2005-04-30:* Post-Doc at Department of Theoretical Chemistry, School of Biotechnology, KTH.

*Leave of absence:*

*2009-04-01-2009-09-30:* Leave of absence due to research visit to Osaka University, Japan.

*2008-06-01-2008-08-31:* Leave of absence due to research visit to Centre for Theoretical and Computational Chemistry, Tromsø, Norway.

**Other information:**

2009 - now: Member of executive committee of KTH Computational Science and Engineering Centre (<http://www.kcse.kth.se/>).

## Degrees and Education

**Academic degrees:**

*2004:* Doctor of Philosophy, Department of Theoretical Chemistry, School of Biotechnology, KTH, Sweden.

*2003:* Licentiate of Philosophy, Department of Theoretical Chemistry, School of Biotechnology, KTH, Sweden.

*2002:* Master Degree in Physics (Cum Laude), Faculty of Fundamental Sciences, Kaunas University of Technology, Kaunas, Lithuania.

## **Brief account of my research efforts:**

I have been working on development and applications of density functional theory (DFT) methods since my studies for Master Degree in Physics (research project "Relativistic calculations of electronic g-tensors of organic radicals", defended in 2002). More specifically, over the last 8 years my research has focused mostly on the two main topics: development of density functional response theory methods for calculations of molecular properties, and applications of these methods to the evaluation of spin-Hamiltonian parameters encountered in magnetic resonance spectroscopy. Recently, I have diversified my research by venturing into simulations of optical and magnetic properties of molecules in complex environments (solvents, proteins, etc.) using multiscale quantum chemistry/molecular dynamics (QM/MD) approaches. In the following I will give a brief account of my research efforts on each of these research directions:

- ***Development of density functional response theory.***

Since the beginning of my scientific carrier I have been involved in development of density functional theory methods for computation of molecular properties and I am one of the main authors of the DFT part of the DALTON quantum chemistry program. I formulated and implemented spin-restricted density functional response theory for evaluation of linear and non-linear properties of paramagnetic molecules. This development made it possible for the first time to perform computations of various non-linear optical, mixed and magnetic properties in open-shell systems using an analytical approach and it significantly extended the capabilities of DFT methods for investigations of paramagnetic compounds. In addition to this, the spin-restricted form of DFT response is by its inherit design free from spin-contamination problems, which plague conventional unrestricted DFT methods and therefore provide more consistent description of various molecular properties. My spin-restricted DFT response formalism has over the last years been successfully applied to investigate various static and dynamics molecular properties of open-shell molecules.

Apart from its significance for actual molecular property calculations, the spin-restricted DFT response formalism has also been important as the basic platform for development of more sophisticated DFT methods. Among such methods, I would like to mention two approaches which I have developed during recent years and which are most representative of my research efforts in the area of density functional theory. The first approach is a restricted-unrestricted formalism, which allows to account for the spin-polarization effects in spin-restricted calculations of linear and non-linear properties. This is accomplished by constructing a variational energy functional with respect to singlet and triplet orbital rotations using the Lagrangian multipliers method. This approach make possible a rigorous evaluation of hyperfine coupling constants and other electronic spin dependent properties within spin-restricted DFT response and is the only viable alternative to unrestricted DFT in systems with heavy spin-contamination, like many transition metal complexes.

The second approach, which I would like to highlight, is the general spin adapted formulation of density functional response theory, which allows to treat the excitations of different multiplicities on equal footing in DFT response computations and which provides the pathway for evaluation of various complex spin-dependent properties, like zero-field splitting constants. Furthermore, it opens the doors for an approximated treatment of multi-electron processes in DFT and a rigorous (from theoretical point of view) description of low spin states of molecules in DFT. From the above achievements of mine in development of density functional theory methods, it follows naturally that I have been focusing on treatment and description of the electronic spin-dependent properties and perturbations within DFT. I focus on open-shell systems, which still remain problematic for conventional density functional theory methods.

- ***Spin-Hamiltonian parameters in EPR and NMR spectroscopy.***

In this research field I have worked on the development of new computational schemes for determination of EPR and NMR spin-Hamiltonian parameters (nuclear shielding constants, electronic g-tensors and others) in open-shell molecules and have actively applied the developed schemes to study organic radicals and paramagnetic transition metal complexes important in various biochemical processes. On the development side, I worked on the methodological aspects of theory and designed computational schemes for evaluation of spin-Hamiltonian parameters based on my spin-restricted DF-RT formalism. In the domain of NMR spectroscopy, I proposed a tractable computational scheme for evaluation of nuclear shielding constants in paramagnetic molecules, which can be used at both the *ab initio* and DFT levels of theory. The proposed methodology has successfully been employed in investigations of organic radicals. Based on the results of these investigations, I showed that the common practice of using the so-called "most similar" diamagnetic compound as reference to evaluate contact shifts in interpretation of experimental data can introduce significant errors and that in general a more sophisticated analysis procedure, which involves quantum chemical calculations, is required for reliable interpretation of NMR measurements. This finding I consider one of the most important of my contributions to NMR spectroscopy of paramagnetic compounds. In the related field of EPR spin Hamiltonian parameters I have proposed several schemes based on my spin-restricted DFT response and restricted-unrestricted approaches for evaluation of electronic g-tensors and hyperfine coupling constants, which go beyond contemporary unrestricted DFT methods in account of both the relativistic effects and environmental effects. Among these methods, I would like to mention one particular approach, namely a degenerate perturbation theory based methodology for evaluation of electronic g-tensors in molecules with doublet ground states, which takes into account higher order relativistic corrections than done in typical electronic g-tensor approaches and that allows to obtain a good quality description of electronic g-tensors in parity with two- or four- component DFT methods. On the application side, I have been working on benchmarking of performance of my computational schemes as well as on investigations of EPR parameters of various paramagnetic copper and vanadium complexes of biological importance. In summary, in this research area I have worked on both with development of computational methods and with their applications to outstanding problems of NMR and EPR spectroscopy of biological systems.

- ***Modeling of molecular properties in complex environments.***

The third research area in which I with co-workers are involved in is simulations of optical and magnetic properties of molecules in solution or protein environments using combined QM/MD approaches. In this field my research is focused along two main directions: simulations of optical properties of solvated chromophores and modeling of nuclear shielding enhancement by paramagnetic molecules, like oxygen or contrast agents, in solution and protein environment. Despite the different properties targeted, the goal of these two research directions is the same, namely to identify environmental factors and "structure to property" relationships, which can be exploited in designing optimal paramagnetic contrast agents or optical or magnetic markers in biological applications.

### **List of publications:**

1. A. Tamulis, Z. Rinkevicius, V. Tamulis, J. Tamuliene, S. P. Karna and C. M. Stickley, "Ab Initio Quantum Chemical Design of Photoactive Molecular Logical Devices", *Nonlinear Optics* vol. 27 (2001), pp. 385-393.
2. A. Tamulis, J. Tamuliene, M. L. Balevicius and Z. Rinkevicius, "Ab Initio Quantum Chemical Search of Per Linear Transition State of Azo-Dye Molecules and Design of Molecular Logical Machines", *Nonlinear Optics* vol. 27 (2001), pp. 481-488.

3. K. Neyman, D. I. Ganyushin, Z. Rinkevicius and N. Rösch, "Hydrogen-bonding effects on electronic g-tensors of semiquinone anion radicals: relativistic density functional investigation", *Int. J. Quant. Chem.* vol. 90 (2002), pp. 1404-1413.
4. Z. Rinkevicius, J. Vaara, L. Telyatnyk and O. Vahtras, "Calculations of nuclear magnetic shielding in paramagnetic molecules", *J. Chem. Phys.* vol. 118 (2003), pp.2550-2561.
5. Z. Rinkevicius, I. Tunell, P. Salek, O. Vahtras and H. Ågren, "Restricted density functional theory of linear time-dependent properties in open-shell molecules", *J. Chem. Phys.* vol. 119 (2003), pp. 34-46.
6. Z. Rinkevicius, L. Telyatnyk, P. Salek, O. Vahtras and H. Ågren, "Restricted density functional linear response theory calculations of electronic g-tensors", *J. Chem. Phys.* vol.119 (2003), pp. 10489-10496.
7. I. Tunell, Z. Rinkevicius, O. Vahtras, P. Salek, T. Helgaker and H. Ågren, "Density functional theory of nonlinear triplet response properties with applications to phosphorescence", *J. Chem. Phys.*, vol. 119 (2003), pp. 11024-11034.
8. B. Minaev, O. Loboda, Z. Rinkevicius, O. Vahtras, H. Ågren, "Fine- and hyperfine-structure in three low-lying  $3\Sigma^+$  states of molecular hydrogen", *Mol. Phys.* vol. 101 (2003), pp. 2335-2346.
9. A. Tamulis, J. Tamuliene, M. L. Balevicius, Z. Rinkevicius and V. Tamulis, "Quantum mechanical studies of intensity in electronic spectra of fluorescein dianion and monoanion forms", *Struct. Chem.* vol. 14 (2003), pp. 643-648.
10. G. P. Berman, F. Borgonovi, Z. Rinkevicius and V. I. Tsifrinovich, "Single-spin measurements for quantum computation using magnetic resonance force microscopy", *Superlattices and Microstructures* vol. 34 (2003), pp. 509-511.
11. L. Telyatnyk, J. Vaara, Z. Rinkevicius and O. Vahtras, "Influence of Hydrogen Bonding in the Paramagnetic NMR Shieldings of Nitronyl Nitroxide Derivative Molecules", *J. Phys. Chem. B.* vol. 108 (2004), pp. 1197-1206.
12. Z. Rinkevicius, L. Telyatnyk, K. Ruud and O. Vahtras, "Electronic g-tensors of solvated molecules using the polarizable continuum model", *J. Chem. Phys.* vol.121 (2004), pp. 5051-5060.
13. Z. Rinkevicius, L. Telyatnyk, O. Vahtras and H. Ågren, "Density functional theory for hyperfine coupling constants with the restricted-unrestricted approach", *J. Chem. Phys.* vol. 121 (2004), pp. 7614-7623.
14. P. Cronstrand, Z. Rinkevicius, Y. Luo, and H. Ågren, "Time-dependent density-functional theory calculations of triplet-triplet absorption", *J. Chem. Phys.* vol. 122 (2005), 224104.
15. C. I. Oprea, Z. Rinkevicius, O. Vahtras, H. Ågren and K. Ruud, "Density functional theory study of indirect nuclear spin-spin coupling constants with spin-orbit corrections", *J. Chem. Phys.* vol. 123 (2005), 014101.
16. L. Frediani, Z. Rinkevicius and H. Ågren, "Two-photon absorption in solution by means of time-dependent density-functional theory and the polarizable continuum model", *J. Chem. Phys.* vol. 122 (2005), 244104.
17. Z. Rinkevicius, L. Telyatnyk and O. Vahtras, "Restricted density functional response theory for open-shell systems" in *Advances in Quantum Chemistry*, Eds. J.~R.~Sabin and E.~Brändas, vol. 50 (2005), pp. 271-288.
18. C. I. Oprea, L. Telyatnyk, Z. Rinkevicius, O. Vahtras and H. Ågren, "Time-dependent density functional theory with the generalized restricted-unrestricted approach", *J. Chem. Phys.* vol. 124 (2006), 174103.
19. E. Rudberg, P. Salek, Z. Rinkevicius and H. Ågren, "Heisenberg exchange in dinuclear manganese complexes: A density functional theory study", *J. Chem. Theory and Comput.* vol. 4 (2006), pp.981-989.

20. J. Tamuliene, Z. Rinkevicius and A. Tamulis, "Investigations of neutral radical molecules suitable for quantum information processing", *Lit. J. Phys.* vol. 47 (2007), pp. 137-142.
21. K. J. de Almeida, Z. Rinkevicius, H. W. Hugosson, A. C. Ferreira and H. Ågren, "Modeling of EPR parameters of copper(II) aqua complexes", *Chem. Phys.* vol. 332 (2007), pp. 176-187.
22. O. Vahtras and Z. Rinkevicius, "General excitations in time-dependent density functional theory", *J. Chem. Phys.* vol. 126 (2007), 114101.
23. G. Tu, Z. Rinkevicius, O. Vahtras, H. Ågren, U. Ekström, P. Norman and V. Carravetta, "Self-interaction-corrected time-dependent density-functional-theory calculations of x-ray-absorption spectra", *Phys. Rev. A* vol. 76 (2007), 022506.
24. Z. Rinkevicius, P. C. Jha, C. I. Oprea, O. Vahtras and H. Ågren, "Time-dependent density functional theory for non-linear properties of open-shell systems", *J. Chem. Phys.* vol. 127 (2007), 114101.
25. S. Gavriluk, S. Polyutov, P. C. Jha, Z. Rinkevicius, H. Ågren and F. Gel'mukhanov, "Many-photon dynamics of photobleaching", *J. Phys. Chem. A* vol. 111 (2007), pp. 11961-11975.
26. J. C. Liu, Y. Velkov, Z. Rinkevicius and F. Gel'mukhanov, "Resonant inelastic X-ray Raman scattering induced by Rabi flopping of core holes", *Chem. Phys. Lett.* vol. 453 (2008), pp. 117-121.
27. J. C. Liu, Y. Velkov, Z. Rinkevicius and F. Gel'mukhanov, "Symmetry-forbidden x-ray Raman scattering induced by a strong infrared-laser field", *Phys. Rev. A* vol. 77 (2008), 043405.
28. P. C. Jha, Z. Rinkevicius, H. Ågren, P. Seal and S. Chakrabarti, "Searching of potential energy curves for the benzene dimer using dispersion-corrected density functional theory", *Phys. Chem. Chem. Phys.* vol. 19 (2008), pp. 2715-2721.
29. X. Li, Z. Rinkevicius, Y. Tu, H. Tian and H. Ågren, "Nuclear Magnetic Shielding of the <sup>113</sup>Cd(II) Ion in Aqua Solution: A Combined Molecular Dynamics/Density Functional Theory Study", *J. Phys. Chem. B.*, vol. 112 (2008), pp. 11347-11352.
30. Z. Rinkevicius, K. J. de Almeida and O. Vahtras, "Density functional restricted-unrestricted approach for nonlinear properties: Application to electron paramagnetic resonance parameters of square planar copper complexes", *J. Chem. Phys.* vol. 129 (2008), 064109.
31. Z. Rinkevicius, K. J. de Almeida, C. I. Oprea, O. Vahtras, K. Ruud and H. Ågren, "Degenerate perturbation theory for electronic g tensors: leading-order relativistic effects", *JCTC* vol. 4 (2008), pp. 1810-1828.
32. Z. Rinkevicius, O. Vahtras, and H. Ågren, "Time-dependent closed and open-shell density functional theory from the perspective of partitioning techniques and projections", *Journal of Molecular Structure: THEOCHEM*, vol. 914 (2009), pp. 50-59.
33. P. C. Jha, Z. Rinkevicius, H. Ågren, "Spin multiplicity dependence of nonlinear optical properties", *Chem. Phys. Chem.* vol. 10 (2009), pp. 817-822.
34. N. Arul Murugan, Z. Rinkevicius and H. Ågren, "Solvent Dependence on Bond Length Alternation and Charge Distribution in Phenol Blue: A Car-Parrinello Molecular Dynamics Investigation", *J. Phys. Chem. A* vol. 113 (2009), pp. 4833-4839.
35. P. C. Jha, Z. Rinkevicius, H. Ågren, "Modeling two photon absorption cross-sections of open shell systems", *J. Chem. Phys.*, vol. 130 (2009), 014103.
36. K. J. de Almeida, N. Arul Murugan, Z. Rinkevicius, H. W. Hugosson, O. Vahtras, A. Cesar and H. Ågren, "Conformations, structural transitions and visible near infrared absorption spectra of four-, five- and six-coordinated Cu(II) aqua complexes", *Phys. Chem. Chem. Phys.* vol. 11 (2009), pp. 508 - 519.
37. N. Arul Murugan, Z. Rinkevicius, H. Ågren, "Modeling solvatochromism of Nile red in water", *Int. J. Quantum Chem.*, vol. XXX (2010), pp. XXX.

38. Z. Rinkevicius and H. Ågren, "Spin-flip time dependent density functional theory for singlet-triplet splittings in  $\sigma,\sigma$ -biradicals", Chem. Phys. Lett., vol. 491 (2010), pp. 132-135.
39. Z. Rinkevicius, O. Vahtras, and H. Ågren, "Spin-flip time dependent density functional theory applied to excited states with single, double or mixed electron excitation character", J. Chem. Phys., vol. 133 (2010), pp. 114104.
40. N. Arul Murugan, P. Jha, Z. Rinkevicius, K. Ruud, H. Ågren, "Solvatochromic shift of phenol blue in water from a combined CPMD-QM/MM and Zindo approach", J. Chem. Phys., vol. 132 (2010), pp. 234508.
41. Z. Rinkevicius, J. Autschbach, A. Baev, M. Swihart, H. Ågren and P.N. Prasad, "Novel Pathways for Enhancing Nonlinearity of Organics Utilizing Metal Clusters", J. Phys. Chem. A, vol. 114 (2010), pp. 7590-7594.
42. K. J. de Almeida. Z. Rinkevicius, O. Vahtras, A. Cesar and H. Ågren, "Modelling of the Visible Absorption Spectra of Copper(II) Acetylacetonate by Density Functional Theory", Chem. Phys. Lett., vol. 492 (2010), pp. 14-18.
43. N.A. Murugan, J. Kongsted, Z. Rinkevicius, K. Aidas and H. Ågren, "Modeling the structure and absorption spectra of stilbazolium merocyanine in polar and non-polar solvents using hybrid QM/MM techniques", J. Phys. Chem. B, vol. XXX (2010), pp. XXX.
44. M. Linares, S. Stafström, Z. Rinkevicius, H. Ågren and P. Norman, "Complex polarization propagator approach in the restricted open-shell self-consistent field approximation: The near K-edge X-ray absorption fine structure spectra of allyl and copper phthalocyanine", J. Phys. Chem. B, vol. XXX (2010), pp. XXX.
45. N.A. Murugan, J. Kongsted, Z. Rinkevicius, and H. Ågren, "reak-down of the "first hyperpolarizability/ bond-length alternation parameter" relationship", Proc. Natl. Acad. Sci. USA, vol. 107 (2010), pp. 16453.
46. X. Chen, F. Ying, Z. Rinkevicius, O. Vahtras, and Hans Ågren, "Restricted-unrestricted density functional theory for hyperfine coupling constants: vanadium complexes ", submitted to Chem. Phys.
47. X. Chen, Z. Rinkevicius, Z. Cao, K. Ruud, and Hans Ågren, "Zero-point vibrational corrections to isotropic hyperfine coupling constants in polyatomic molecules", submitted to Phys. Chem. Chem. Phys.

### Other scientific achievements:

#### *Active participation in national and international conferences (last five years):*

- Excited State Processes in Electronic and Bio Nano-Materials, Santa Fe, USA, 2005.
- CERC3 Young Chemists' Workshop (YCW) "Modeling of Complex Systems" in Perugia, Italy, 2008. (invited speaker)
- EU/India network MONAMI meeting, MPI, Stuttgart, Germany, 2009.
- Diradicals and Multiradicals: Theory and Experiment, Namur, Belgium, 2009.
- Multiscale Modeling and Simulation in Science, Stockholm, Sweden, 2009.
- Annual meeting of KTH Computational Science and Engineering Centre, Lovik, Lidingö, 2009. (organizer)
- DALTON quantum chemistry program developers meeting, Oslo, Norway, 2010.

#### *Research visits:*

- 2005, September-October: Complex Systems Group T-13, Los Alamos National Laboratory (USA), host dr. G. Berman. Projects ``Quantum computation using self-

assembled molecular spin arrays" and "Molecular Observation, Spectroscopy and Imaging using Cantilevers".

- 2008, June-September: The Centre for Theoretical and Computational Chemistry, Tromsø, Norway, host prof. K. Ruud. Project "Vibrational averaging of the EPR properties".
- 2009, April-September: University of Osaka, Osaka, Japan, host prof. M. Nakano. Project "Non-linear optical properties of biradicals".

*Development of quantum chemistry codes:*

I am co-author of DALTON quantum chemistry program (<http://www.daltonprogram.org>) and one of main contributions to its density functional theory code.