List of publications

Jiří Pittner

Monography chapters

1. Bonačić-Koutecký V., Pittner J., Fuchs C., Fantucci P., and Koutecký J.:
Quantum Chemical Investigation of Absorption Spectra of Small Alkali Metal Clusters; Molecular Dimensionality Transition (2D–3D),
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Invited talks:

1. 3-rd Central European Symposium on Quantum Chemistry, Tihany, Hungary (2004) *Recent Advances in the Multireference Brillouin-Wigner Coupled Clusters Method*

2. 45-th Sanibel Symposium, St. Simons Island, Georgia, USA (2005): *Recent Advances in the Multireference Brillouin-Wigner Coupled Clusters Method*

3. 13-th European Seminar on Computational Methods in Quantum Chemistry, Smolenice, Slovakia (2005): *Recent Advances in the Multireference Brillouin-Wigner Coupled Clusters Method*

4. 5-th Central European Symposium on Quantum Chemistry, Zakopane, Poland (2006): *Multireference Brillouin-Wigner Coupled Cluster Method with Connected Triples*

5. 6-th Congress of the International Society for Theoretical Chemical Physics, Vancouver, Canada, July 2008: *An alternative formulation of the Mukherjee's State-Specific MRCC Theory with Simpler Coupling Terms*

6. Theory and Applications of Computational Chemistry (TACC) 2008, Shanghai, China, September 2008: *Efficient techniques for non-adiabatic molecular dynamics*

7. 3rd Japan-Czech-Slovak symposium, Bratislava 2009: *State-Specific Multireference Coupled Cluster Methods with Triexcitations: Brillouin-Wigner, Mukherjee, and Uncoupled Mukherjee Approaches.*

8. Eighth International Conference of Computational Methods in Sciences and Engineering (ICCMSE), Kos, 2010: *Recent Progress in Multireference Hilbert-space coupled cluster methods: triexcitations and R12 explicit correlation*

9. American Chemical Society Spring Meeting, Anaheim 2011: *Quantum computing applied to calculation of molecular energies*

10. The Seventh Congress of the International Society for Theoretical Chemical Physics (ISTCP-VII), Tokyo, 2011: *Towards quantum chemistry on quantum computers*

11. Recent advances in many electron theories - II (RAMET-II), Puri (India), 2011: *Recent Progress in Multireference Hilbert-space coupled cluster methods: Explicit correlation, Massively Parallel Implementation, and USS Corrections*

12. Central European Symposium on Theoretical Chemistry (CESTC 2012), Mariapfarr, 2012: *Multireference coupled cluster methods with explicit correlation*

13. The Eigth Congress of the International Society for Theoretical Chemical Physics (ISTCP-VIII), Budapest, 2013 *Recent Progress in Multireference Hilbert-Space Coupled Cluster Methods*

14. 5-th JCS Symposium on theoretical chemistry, Nara 2013 *Molecular dynamics with non-adiabatic and spin-orbit effects*

15. WATOC 2014, Santiago de Chile, 2013 *Molecular dynamics with non-adiabatic and spin-orbit effects*

16. QESC 2015 - ICQC 2015 Satellite symposium: Novel Computational Methods for Quantitative Electronic Structure Calculations, Kobe, June 2015

17. Theory and Applications of Computational Chemistry (TACC) 2016, Seattle 2016

18. World Association of Theoretically Oriented Chemists (WATOC) 2017, Munich, Germany, September 2017

19. Sanibel Symposium, St. Simons Island, February 2019

20. 10th Triennial Congress of the International Society for Theoretical Chemical Physics (ISTCP), Tromso, July 2019

21. Warsaw Molecular Electronic Structure conference, online (University of Warsaw), September 2020

22. Torun Astrophysics, theoretical Spectroscopy, and Quantum chemistry, mini-symposium, online (University of Torun), October 2020

23. Tensor product methods for strongly correlated molecular systems, online (Max Planck Institute of Complex Systems, Dresden) March 2021

24. STC2021 - 57th Symposium on Theoretical Chemistry, online (University of Wuerzburg), September 2021

25. QSCP2022 - 25th International Workshop on Quantum Systems in Chemistry, Physics and Biology, Torun, Poland, June 2022

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1. Development of the MR BWCCSD method, Grant Agency of the Czech Republic, 2000–2002
2. Analytic gradient of the MR BWCCSD method, Grant Agency of the Czech Republic, 2004–2006
3. MR BWCC method with connected triple excitations, Grant Agency of the Academy of Sciences of the Czech Republic, 2004–2007
4. Computer-aided implementation of multireference coupled cluster methods, Grant Agency of the Czech Republic, 2007-2010
5. Efficient methods for ab-initio non-adiabatic molecular dynamics, Grant Agency of the Academy of Sciences of the Czech Republic, 2008-2011
6. Quantum Chemistry on Quantum Computers, Grant Agency of the Czech Republic, 2008-2012
7. Explicitly correlated multireference coupled cluster methods, Grant Agency of the Czech Republic, 2011-2015
8. Ab initio molecular dynamics with non-adiabatic and spin-orbit effects applied to time-dependent fluorescence, Grant Agency of the Czech Republic, 2012-2016
9. Hilbert-space multireferenční coupled cluster metody, jejich paralelní implementace a aplikace na excitované stavy, MŠMT-AMVIS, 2013-2015.
10. DMRG-based externally corrected coupled cluster methods, Czech Science Foundation, 2016-2018
11. Relativistic DMRG-based externally corrected coupled cluster methods, Czech Science Foundation, 2018-2020
12. New coupled cluster methods externally corrected by DMRG: Implementation for new generation of supercomputers and application to transition metal complexes, Czech Ministry of Education, 2017-2020
13. Time evolution of conjugated systems in excited states by surface hopping nonadiabatic molecular dynamics, (co-PI), Czech Science Foundatuion, 2019-2021