Jacek Jakowski
National Institute for Computational Sciences,
JICS-ORNL, University of Tennessee
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I am interested in development and implementation computational chemistry methods for GPU and high-performance computing architectures.
Current scientific interest focuses on the development of efficient large scale quantum dynamics methods based on tight-biding density functional approaches for electronic structures and Bohmian formalism of quantum mechanics for the application in energy research and modeling nanoscale materials.

Education/Training:

University of Warsaw, Theoretical Chemistry	Ph.D. 2002
University of Warsaw, Theoretical Chemistry	M.Sc 1996

Research and Professional Experience:

since 2016 Staff scientist, Oak Ridge National Laboratory, Oak Ridge, TN
2010-2016 Computational Scientist, Joint Institute of Computational Sciences, University of Tennessee & Oak Ridge National Laboratory, Oak Ridge, TN
2007- 2010 Research Associate, Emory University, Atlanta, GA
2004 -2007 Postdoctoral Research Associate, Indiana University, Bloomington, IN
2002- 2004 Postdoctoral Research Associate, University of Utah, Salt Lake City
1998- 2002 Assistant Professor of Physical Chemistry, Medical University of Warsaw, Faculty of Pharmacy, Warsaw, Poland

Professional Activities, Honors and Awards:

2015 Wiley Visiting Scientist, Environmental Molecular Sciences Laboratory, PNNL
2014 CNMS/ORNL distinguished scientific paper
2008-2009 Advanced programming courses: (a) operating system programming, (b) parallel processing; Math & Computer Science Dept. ; Emory University
2008 Nvidia's Professor Partnership Program (with Keiji Morokuma)
2002 Distinguished Ph.D. University of Warsaw
1998 Electoral College fellow
1997-1999 President of Ph.D. student body, Department of Chemistry, University of Warsaw

Synergistic Activities:

1 Conference (co)organized: (1) *Second Annual EPSCoR Workshop: Modeling Advanced Materials, Systems Biology and Alternative Energy Sources*", Knoxville, October 10-12/2011, (2) "*Electronic Structure Calculation Methods on Accelerators*", Oak Ridge/Knoxville, February 5-8,2012, (3) organizing committee Xsede 2014, Atlanta.

2 Referee for the (a) Computer Physics Communications, (b) Materials Chem. Physics, (c) Nuclear Instruments and Methods in Physics Research B, (d) International Journal of Quantum Chemistry, (e) Molecular Physics (f) Journal of Chemical Theory and Computations, (g) Concurrency and Computations, (h) Modern Physics Letters B (i) GPU computing Gems, (j) DOE INCITE (computational readiness) and ASCR proposals (k) NSF Xsede, (l) Shota Rustaveli National Science Foundation of Georgia

3 Lecturer at several HPC national and international workshops. Some invited talks at International workshops: (a) *DFTB Thai Summer School in Computational Chemistry*, Bangkok, Oct.2010, (b) "*Large Scale Computer Simulations*", Aachen/Julich, Germany, March 2011, (c) IRSES, Nagoya, March 2012, (d) 53rd Sanibel Symposium, St. Simons Island, GA, Feb. 17-22, 2013, "*Modeling Materials at the Nanoscale- Quantum Dynamical Perspective*" (invited plenary lecture), (e) 2013 Telluride Science Research Center Conference on Advances In Photoreactions: When Spin-Orbit

Coupling, Optical Excitation, and Motion of Nuclei are of Equal Importance, Telluride, CO, June 22-25, 2013, *"Modeling Materials at the Nanoscale",* (f) *Summer School of Physics*, Jacobs University, Bremen, Germany, June 16-27, 2014

4 Member of (a) American Chemical Society, (b) International Society for Theoretical Chemical Physics, (c) American Association for the Advancement of Science

5 Mentoring 14 undergraduate and graduate intern students during years 2010-2015; and two faculty in the role of XSEDE campus champions

Collaborators:

Keiji Morokuma (Emory University), Stephan Irle (Nagoya University), Sophya Garashchuk (University of South Carolina), Steven Stuart (Clemson University), Poul Jorgensen (Aarhus University), Predrag Krstic (Joint Institute for Computational Science), Bobby Sumpter (Oak Ridge National Laboratory), Jingson Huang (CNMS/ORNL), Vitaly Rassolov (University of South Carolina), Grzegorz Chalasinski (University of Warsaw), Jack Simons (University of Utah)

Graduate and Postdoctoral Advisors: Keiji Morokuma (Emory University), Srinivasan Iyengar (Indiana University), Jack Simons (University of Utah), Grzegorz Chalasinski (University of Warsaw, Poland)

Conference (co)organized:

1. "*Second Annual EPSCoR Workshop: Modeling Advanced Materials, Systems Biology and Alternative Energy Sources*", Knoxville, October 10-12/2011. http://www.nics.tennessee.edu/EOT/Epscor,
2. "*Electronic Structure Calculation Methods on Accelerators*", Oak Ridge/Knoxville, February 5-8, 2012 http://www.nics.tennessee.edu/feb-2012-accelerator-workshop
3. XSEDE 14, "Accelerating Discovery in Scholarly Research" (Science Track), technical committee member, July 13-18/2014

Book Chapters:

1 J. Huang, J. Jakowski, A. Beste, J. Younker, A. Vazquez-Mayagoitia, E. Cruz-Silva, M. Fuentes-Cabrera, A. Lopez-Benzanilla, V. Meunier, Bobby G. Sumpter,"*Advancing Understanding and Design of Functional Materials through Theoretical and Computational Chemical Physics",* in J. Leszczynski, M. K. Shukla, Eds. "*Practical Aspects of Computational Chemistry II: An Overview of the Last Two Decades and Current Trends*", Springer-European Academy of Sciences (2012). ISBN 978-94-007-0922-5

2 J. Jakowski, S. Irle, K. Morokuma, "*Quantum Chemistry: propagation of Electronic Structure on GPU*" chapter 5, pp. 59-74, in "*GPU Computing Gems. Emerald edition*", edited by Wen-mei Hwu, Morgan Kauffman (Elsevier), 2011, ISBN 978-0-12-384988-5, [doi: 10.1016/B978-0-12-384988-5.00005-X]

Publications:

1. L. Wang, J. Jakowski, S. Garashchuk, B.G. Sumpter, "*Understanding how Isotopes Affect Charge Transfer in P3HT/PCBM: A Quantum Trajectory-Electronic Structure Study with Nonlinear Quantum Correction*", J. Chem. Theory and Comput. (submitted)
2. S. Garashchuk, J. Jakowski, V. Rassollov *Approximate quantum trajectory dynamics for reactive processes in condensed phase* Molecular Simulation., 41,86-106 (2015), DOI: 10.1080/08927022.2014.907493

3. James Mazucca, Sophya Garashchuk, Jacek Jakowski, "The effect of local substrate motion on quantum hydrogen transfer in soybean lipoxygenase-1 modeled with QTES-DFTB dynamics". Chem. Phys. Lett, 613, 104-109 (2014) [doi: 10.1016/j.cplett.2014.08.006]
4. Lei Wang, Jacek Jakowski, Sophya Garashchuk, "Adsorption of a Hydrogen Atom on a Model Graphene Examined with a Quantum Trajectory/Electronic Structure Dynamics", J. Physical Chemistry C, *118* , pp 16175–16187 (2014) [doi: 10.1021/jp503261k]
5. Dulma Nugawela, Steven Stuart and Jacek Jakowski, "Highly Energetic Collisions of Xe with Fullerene Clusters", XSEDE14 Atlanta, Conference Proceedings, ACM digital library, 2014 [doi: 10.1145/2616498.2616514]
6. Lei Wang, James Mazzuca, Sophya Garashchuk and Jacek Jakowski , "The hybrid Quantum Trajectory/Electronic Structure DFTB-based approach to Molecular Dynamics", XSEDE14, Atlanta, Conference Proceedings, ACM digital library, 2014 (http://dl.acm.org/citation.cfm?id=2616503) [doi 10.1145/2616498.2616503]
7. Ming Shao, Jong Keum, Jihua Chen, Youjun He, Wei Chen, James F. Browning, Jacek Jakowski, Bobby G. Sumpter, Ilia N. Ivanov, Ying-Zhong Ma, Christopher M. Rouleau, Sean C. Smith, David B. Geohegan, Kunlun Hong, Kai Xiao*, The isotopic effects of deuteration on the optoelectronic properties of conducting polymers,* Nature Comm. 5, 4180 (2014) [doi: 10.1038/ncomms4180]
8. S. Garashchuk, J. Jakowski, L. Wang and B. Sumpter. *Quantum Trajectory-Electronic Structure Approach for Exploring Nuclear Effects in the Dynamics of Nanomaterials.* J. Chem. Theory and Comput. 9, 5221-5235 (2013). [doi: 10.1021/ct4006147]
9. Kasper Kristensen, Thomas Kjaergaard, Ida-Marie Hoyvik, Patrick Ettenhuber, Poul Jorgensen, Branislav Jansik, Simen Reine, Jacek Jakowski, *The Divide-Expand-Consolidate MP2 scheme goes massively parallel*, Molecular Physics , 111, 1196-1210 (2013) [doi:10.1080/00268976.2013.783941]
10. P.S. Krstic, J.P. Allain, C. Taylor, J. Dadras, S. Maeda, K. Morokuma, J. Jakowski and A. Allouche, C. H. Skinner,"*Deuterium uptake in magnetic-fusion devices with lithium-conditioned carbon walls*", Phys. Rev. Lett. 110, 105001 (2013) [doi: 10.1103/PhysRevLett.110.105001]
11. Kasper Kristensen, Ida-Marie Hoyvik, Branislav Jansik , Poul Jorgensen, Thomas Kjargaard, Simen Reine, Jacek Jakowski, "*Pushing the frontiers of accurate quantum mechanical calculations*", Phys. Chem. Chem. Phys.14,15706-15714 (2012),[doi:10.1039/C2CP41958K]
12. James Mazzuca, Sophya Garashchuk, Jacek Jakowski, "*Description of proton transfer in soybean lipoxygenase-1 employing approximate quantum trajectory dynamics*". Chem. Phys. Lett, 542, 153-158 (2012) [doi:10.1016/j.cplett.2012.06.019]
13. Jacek Jakowski, B. Hadri, S. J. Stuart, P. Krstic, S. Irle, D. Nugawela, S. Garashchuk, "*Optimization of density functional tight-binding and classical reactive molecular dynamics for high-throughput simulations of carbon materials*", XSEDE'12, Conference proceedings, ACM, pp. 36:1-7, 2012, [doi:10.1145/2335755.2335832]
14. J. Jakowski, S. Irle, B. Sumpter, K. Morokuma, "*Modeling charge transfer in fullerene collisions via real-time electron dynamics*", J. Phys. Chem. Lett, 3,1536-1542 (2012), [doi:10.1021/jz3004377]
15. J. Jakowski, S. Irle, K. Morokuma, "*Time–dependent quantum dynamical simulations of C_2 condensation under extreme conditions*", Phys. Chem. Chem. Phys. **14**, 6273-6279 (2012) [doi:10.1039/C1CP22035G]
16. R C Ehemann, J Dadras, P R C Kent, J Jakowski, and P S Krstić, "*Detection of hydrogen using graphene*", Nano Research Letters, 2012, **7**:198, [doi: 10.1186/1556-276X-7-198]
17. P. Krstic, J. P. Allain, A. Allouche, J. Jakowski, J. Dadras, C.N. Taylor, Z. Yang, "*Dynamics*

of Deuterium Retention and Sputtering of Li- C-O Surfaces", Fusion Engineering and Design,87, 1732-1736 (2012) [doi:10.1016/j.fusengdes.2011.07.009]

18. J. Jakowski, S. Irle, K. Morokuma, "*Collision-Induced fusion of two C_{60} fullerenes: Quantum chemical molecular dynamics simulations*", Physical Reviews B. vol. **82**, 125443 (2010), [doi:10.1103/PhysRevB.82.125443]
19. J. Jakowski, K. Morokuma, "*Liouville von Neumann Molecular Dynamics*", Journal of Chemical Physics, **130**, 224106 (2009), [doi:10.1063/1.3152120], ,
20. G. Zheng, M. Lundberg, J Jakowski, T. Vreven, M. Frisch, K. Morokuma," *Implementation and Benchmark Tests of the DFTB Method and Its Application in the ONIOM Method*, International Journal of Quantum Chemistry, **109**,1841-1854 (2009) [doi:10.1002/qua.22002]
21. S. S. Iyengar, I. Sumner and J. Jakowski "*Hydrogen tunneling in an enzyme active site: a quantum wavepacket dynamical perspective*". J. Phys. Chem. B **112**, 7601 (2008). [doi: 10.1021/jp7103215]
22. A. Zielinska, K. Paradowska, J. Jakowski, I. Wawer, "*C-13 CP MAS NMR and GIAO-CHF/DFT calculations of flavonoids: Morin, kaempferol, tricin, genistein, formononetin and 3.7-dihydroxyflavone*", J. of Molecular Structure, **873,** 109-116 (2008) [doi:10.1016/j.moistruc.2007.03.009]
23. P. Skurski, M. Sobczyk, J. Jakowski, J. Simons, "*Possible mechanisms for protecting N-C-alpha bonds in helical peptides from electron-capture (or transfer) dissociation*", Int. Journal of Mass Spectroscopy, **265**, 197-212 (2007) [doi: 10.1016/j.ijms.2007.02.001]
24. F. E. Massoth, P. Politzer, P., M.C. Concha, J. S. Murray, J. Jakowski, J. Simons, "*Catalytic hydrodeoxygenation of methyl-substituted phenols: Correlations of kinetic parameters with molecular properties*", J. Phys. Chem. B, 110, 14283-14291 (2006) [doi:10.1021/jp057332g]
25. J. Jakowski, I. Sumner and S. S. Iyengar, "*Computational Improvements to Quantum Wavepacket Ab Initio Molecular Dynamics using a potential-adapted, time-dependent deterministic sampling technique*". Journal of Chemical Theory and Computation **2**, 1203-1219 (2006). [doi: 10.1021/ct600131g]
26. S. S. Iyengar and J. Jakowski, "*Quantum Wavepacket Ab Initio Molecular Dynamics: An approach to study quantum dynamics in large systems*". J. Chem. Phys. 122, 114105 (2005). [doi: 10.1063/1.1871876]
27. D. Maciejewska, J. Jakowski, P. Kleps, G. Chalasinski, "*Conformational analysis of N-benzyl-N-o-tolyl-p-methylbenzene-sulfonamides from dynamic H-1 NMR experiments and theoretical calculations*", J. of Molecular Structure-Theochem, 680, 5-13 (2004) [doi: 10.1016/j.theochem.2004.04.024]
28. J. Jakowski and J. Simons, "*Theoretical Analysis of the Electronic Structure and Bonding Stability of the TCNE Dimer Dianion $(TCNE)_2^{2-}$*", J. Am. Chem. Soc. **125**, 16089-16096 (2003), [doi: 10.1021/ja030240p]
29. J. Jakowski, G. Chalasinski, S. Cybulski, M. M. Szczesniak, "*Modeling of the three-body effects in the Ar_2O^- trimer from ab initio calculations*", J. Chem. Phys, 118, 2731-2747 (2003) [doi: 10.1063/1.1531109]
30. J. Jakowski, G. Chalasinski, J. Gallegos, M. W. Severson, Szczesniak M.M. "*Characterization of Ar_nO^- clusters from ab initio and diffusion Monte Carlo calculations*", J. Chem. Phys. 118, 2748-2759 (2003), [doi: 10.1063/1.1531110]
31. J. Jakowski, G. Chalasinski, M.M. Szczesniak, S.M. Cybulski, "*Modeling of the three-body effects in the neutral trimers in the quartet state by ab initio calculations. H_3^-, Na_3^-, and*

Na_2B", Collection of Czechoslovak Chemm. Communications, 68, 587-626 (2003), [doi: 10.1135/cccc20030587]

32. J. Jakowski, J. Klos, G. Chalasinski, M.W. Severson, M.M. Szczesniak, S. M. Cybulski, "*Structure and energetics of Ar_nNO^- clusters from ab initio calculations*", J. Chem. Phys. 112, 10895-10904 (2000) [doi: 10.1063/1.481730]
33. A. A. Buchachenko, J. Jakowski, G. Chalasinski, M.M. Szczesniak, S. M. Cybulski, "*Ab initio based study of the ArO^- photoelectron spectra: Selectivity of spin-orbit transitions*", J. Chem. Phys. 112, 5852-5865 (2000) [doi: 10.1063/1.481186]
34. J. Jakowski, G. Chalasinski, M. M. Szczesniak, "*Many-body exchange effects in clusters of rare gases with a chromophore: He_2CO_2*", Chem. Phys. 239, 573-591 (1998) [doi: 10.1016/S0301-0104(98)00335-8]

Selected Recent Presentations

1. *CECAM conference*, Development of next generation accurate approximate DFT/B methods, Bremen, Germany, Oct 10-15, 2015 (invited talk) ,"*Quantum Methods for Temporal and Spatial Multiphysics of Nanomaterials*".
2. "Modeling multiphysics processes of nano-scale systems with tight-binding DFT methods", Wiley Seminar, PNNL, Richland, WA, Sept. 25,2015
3. *Beyond Exascale: Qubits for Quantum Computing* Workshop, Oak Ridge, TN, Aug 20-21, 2015, "*Tight-Binding Density Functional Theory (DFT) Methods for Understanding Dynamics in Nanostructures"*
4. *NWChem Workshop & Developer Meeting.* New and Future Directions in Atomistic Simulation & Modeling, Seattle, USA. *Quantum dynamical simulation of nano-materials with tight-binding DFT",* October 27-30, 2014 (invited talk)
5. *248th National ACS Meeting,* San Francisco, "Quantum reaction dynamics of nanoscale materials", August 14, 2014 (contributing talk)
6. WE-Heraeus Physics Summers School 2014, Jacobs University, Bremen, Germany, *"Exploring electron dynamics in real-time: towards the control of electron motion in materials"* June 20, 2014 (invited talk)
7. WE-Heraeus Physics Summers School 2014, Jacobs University, Bremen, Germany, *"Exploring quantum nuclear effects with quantum trajectory electronic structure approach",* June 23, 2014 (invited talk)
8. *APS march meeting,* Solvation, Dynamics, and Reactivity in Complex Environments IV. J. Mazucca, S. Garashchuk, J. Jakowski, *QTES-DFTB dynamics study on the effect of substrate motion on quantum proton transfer in soybean lipoxygenase-1.*
9. 2013 Telluride Science Research Center Conference on Advances In Photoreactions: When Spin-Orbit Coupling, Optical Excitation, and Motion of Nuclei are of Equal Importance, Telluride, CO, June 22-25, 2013, *"Modeling Materials at the Nanoscale"* (invited lecture)
10. 53rd Sanibel Symposium, St. Simons Island, GA, Feb. 17-22, 2013, "*Modeling Materials at the Nanoscale- Quantum Dynamical Perspective*" (invited plenary lecture)
11. "Development of New Quantum Chemical Molecular Dynamics for Materials Science Modeling", XSEDE -ECSS symposium, 04/16/2013
12. Jacek Jakowski, "Computational Advanced Materials Endstation on HPC architectures", at the "Tennessee CyberInfrastructure Symposium" 04/04/2013, TSU, Nashville, (invited talk)
13. "Modeling Advanced Materials. EPSCoR Desktop to Petascale Ecosystem". NCCS/ORNL,

October 31, 2013, (seminar)

14. "*Collision of neutral and charged fullerenes as a prototype on non-equilibrium, non-adiabatic, redox reaction- quantum dynamics simulations*". at the 244th American Chemical Society National Meeting, Philadelphia, PA, Aug 19-23, 2012 (talk)
15. Jacek Jakowski, Steve Stuart, Dulma Nugawela, Bilel Hadri, Sophya Garashchuk, Predrag Krstic, Stephan Irle, Optimization of Density Functional Tight-Binding and Classical Reactive Molecular Dynamics for High-Throughput Simulations of Carbon Materials, Xsede 2012, Chicago, July 16-20, 2012 (contributing talk)
16. Galen Collier, Jill Gemmill, James Von Oehsen, Bhanu Rekepalli, Jacek Jakowski, Starr Hazard, Jerry Ebalunode and Clayton Mccauley, "Education, Outreach, and Training within the Desktop-to-Petascale Ecosystem", Xsede 2012, Chicago, July 16-20, 2012 (poster)
17. "*Electron Transfer and Energy Transfer in Carbon Materials*" at the 14th International Congress of Quantum Chemistry, Boulder, CO, June 25-30, 2012 (poster)
18. "*Real time simulations of electron transfer and energy transfer in carbon materials*", Clemson University, April 8, 2012 (seminar)
19. "*Real time simulations of electron transfer and energy transfer in carbon materials*", at the 2012 meeting of the South Eastern Theoretical Chemistry Association, (SETCA 2012), University of Georgia, Athens, GA, May 17-19, 2012 (talk)
20. "*Electron and energy transfer in carbon materials from quantum dynamics simulations*" at the 1st International Workshop on Computer Simulations of Thermally Excited Molecules and Materials by First Principles (IRSES), Nagoya University, Japan, March 06-08, 2012 (talk)
21. Jacek Jakowski and Bhanu Rekepalli. "Collaborative Research: An EPSCoR Desktop to TeraGrid Ecosystems. Integrating Campus-Based Research with National Cyberinfrastructure", poster presented at 2012 Computing and Computational Sciences Directorate Advisory Committee, ORNL, Oak Ridge, TN, Feb 21-23, 2012 (poster)
22. "*Time-dependent quantum dynamical simulations of C2 condensation under extreme conditions*" at the 7th congress of International Society of Theoretical Chemical Physics/ Tokyo, Waseda University, Japan, Sept.2- 8, 2011 (poster)
23. "*Electronic structure on GPU*" at the "HPC in Chemistry" workshop, Knoxville, TN, Aug 8, 2011 (talk)
24. "*Quantum Dynamical Simulations of Nanoscale Materials. Theory, implementation and simulations" at the "Materials by design*" workshop, organized by CNMS/ORNL, Oak Ridge, TN, Sept 20-22, 2011 (invited talk)
25. "*From fullerenes to nano-devices. Modeling reactions between carbon nano-structures from quantum chemical molecular dynamics simulations*", Xsede 2011, Salt Lake City, July 19, 2011 (talk)
26. "*Liouville von Neumann Molecular Dynamics*" at the GRS/JICS workshop on Large-Scale Computer Simulation. Aachen / Jülich, Germany, March 9-11, 2011 (invited talk)
27. "*Liouville von Neumann Dynamics*" at the "DFTB Thai Summer School in Computational Chemistry", Kasetsart University Kamphaeng Saen Campus, Bangkok, October 11-14, 2010 (invited lecture)
28. "*Liouville-von Neumann dynamics on GPU*", at the 240th National Meeting of the American Chemical Society, Boston, MA, August 22, 2010 (talk)