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I am interested in development and application of computational chemistry and materials science methods for Quantum Processors, GPU, and high-performance computing architectures. Current scientific interest focuses on electronic structure (ground and excited) and dynamics in application to CO_2 capture and conversion, interaction of materials with beam of particles, plasma and light, quantum nuclear effects and dynamics, application of quantum computing in quantum chemistry problems.
Google scholar profile: https://tinyurl.com/jakowski-google

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:

2020	CSED/ORNL Significant Event Award for quantum computing benchmark
2019	UT-Battelle Director's Award to Team Accomplishment
2019	UT-Battelle's Award for Research Accomplishment
2015	Wiley Visiting Scientist, Environmental Molecular Sciences Laboratory, PNNL
2014	CNMS/ORNL distinguished scientific paper
2008	Nvidia's Professor Partnership Program (with Keiji Morokuma)
2002	Distinguished Ph.D. University of Warsaw
1998	Electoral College fellow, University of Warsaw
1997-1999	President of Ph.D. student body, Department of Chemistry, University of Warsaw

Synergistic Activities:

1. Member of (a) American Chemical Society, (b) American Physical Society
2. Referee for major publishing houses including (a) Elsevier, (b) Wiley (c) American Chemical Society (d) Nature-Springer (e) Royal Society of Chemistry (f) American Institute of Physics
3. Panel review member for NSF-XSEDE/ACCESS allocation committee, since 2013

4. Ad Hoc reviewer for (a) National Science Foundation, (b) DOE -INCITE, ALCC, ASCR proposals (c) Shota Rustaveli National Science Foundation of Georgia, (d) ACS PRF,
5. Conferences co-organized: (1) PEARC23: Practice and Experience in Advanced Research Computing, program committee, July 23-27, 2023, (2) "*Second Annual EPSCoR Workshop: Modeling Advanced Materials, Systems Biology and Alternative Energy Sources*", Knoxville, October 10-12/2011. (3) "*Electronic Structure Calculation Methods on Accelerators*", Oak Ridge/Knoxville, Feb. 5-8, 2012, (4) XSEDE 14, "Accelerating Discovery in Scholarly Research" (Science Track), technical committee member, July 13-18/2014

Collaborators: Syed Islam (ORNL), Gonzalo Alvarez (ORNL), Juan-Carlos Idrobo (ORNL), Jerry Berhholc (NCSU), Mina Yoon (ORNL), Tao Yu (University of North Dakota), Panchakepasan Ganesh (ORNL), Jong Keum (ORNL), Jingsong Huang (ORNL), Kunlun Hong(ORNL), Travis Humble (ORNL), Raphael Pooser (ORNL), Keiji Morokuma (Emory University), Stephan Irle (ORNL), Sophya Garashchuk (University of South Carolina), Steven Stuart (Clemson University), Poul Jorgensen (Aarhus University), Predrag Krstic (Stony Brook), Bobby Sumpter (Oak Ridge National Laboratory), Jingsong 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)

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 [DOI:10.1007/978-94-007-0923-2_7]

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. Jordan A Hachtel, Jacek Jakowski, Jingsong Huang, Santa Jansone-Popova, Ilja Popovs, Elizabeth A Richardson, Barbara R. Evans, Peter Rez, Eric V Fromo, "A New Path to Nanoscale Cellular Analysis with Monochromated Electron Energy-Loss Spectroscopy", arXiv:2206.04191 [doi: 10.48550/arXiv.2206.04191]
2. Sachith Wickramasinghe, Alexandria Hoehn, Shehani T. Wetthasinghe, Huina Lin, Qi Wang, Jacek Jakowski, Vitaly Rassolov, Chuanbing Tang, Sophya Garashchuk, "Theoretical examination of the hydroxide transport in cobaltocenium-containing polyelectrolytes", J. Phys. Chem. B (2023), 127, 47, 10129–10141 [doi: 10.1021/acs.jpcb.3c04118]
3. J. Goings, L. Zhao, J. Jakowski, T. Morris and R. Pooser, "*Molecular Symmetry in VQE: A Dual Approach for Trapped-Ion Simulations of Benzene*," 2023 IEEE International Conference on Quantum Computing and Engineering (QCE), Bellevue, WA, USA, 2023, pp. 76-82, [doi: 10.1109/QCE57702.2023.10187.]
4. Gonzalo Alvarez, Ryan Bennink, Stephan Irle, Jacek Jakowski, *Gene Expression Programming for Quantum Computing*, ACM Transactions on Quantum Computing (2023), 4, 27:1-14 [doi: 10.1145/3617691]

5. Jacek Jakowski, Jingsong Huang, Syed Z. Islam, David S. Sholl, "*Quantum Chemical Simulations of CO2 and N2 Capture in Reline, a Prototypical Deep Eutectic Solvent*", J. Phys. Chem. B, (2023), (2023), 127, 8888-8899 [doi: 10.1021/acs.jpcb.3c02174]
6. Shubhangi Shukla, Jacek Jakowski, Sachin Kadian, Roger J. Narayan, "*Computational approaches to delivery of anticancer drugs with multidimensional nanomaterials*", in Computational and Structural Biotechnology Journal, (2023), 21, 4149-4158, [doi: 10.1016/j.csbj.2023.08.010]
7. S. Islam, A. Arifuzzaman, G. Rother, V. Bocharova, R. Sacci, J. Jakowski, J. Huang, I. N. Ivanov, R. R. Bhave, T. Saito, D. Sholl, *A Membrane Contactor Enabling Energy-efficient CO2 Capture from Point Sources with Deep Eutectic Solvents*, Ind. & Eng. Chem. Res. (2023) 62, 10,4455-4465 [DOI: 10.1021/acs.iecr.3c00080]
8. Anthony Yoshimura, Michael Lamparski, Joel Giedt, David Lingerfelt, Jacek Jakowski, Panchapakesan Ganesh, Tao Yu, Bobby G. Sumpter, Vincent Meunier, *Quantum theory of electronic excitation and sputtering by transmission electron microscopy*, Nanoscale, (2023)15, 1053-1067 [DOI: 10.1039/D2NR01018F]
9. Van-Quan Vuong, Caterina Cevallos, Ben Hourahine, Bálint Aradi, Jacek Jakowski, Stephan Irle, Cristopher Camacho, *Accelerating the Density-Functional Tight-Binding Method Using Graphical Processing Units*, J. Chem. Phys. (2023) [DOI: 10.1063/5.0130797]
10. David B. Lingerfelt, Anthony Yoshimura, Jacek Jakowski, Panchapakesan Ganesh, Bobby G. Sumpter, *Extracting Inelastic Scattering Cross Sections for Finite and Aperiodic Materials from Electronic Dynamics Simulations*, J. Chem. Theory and Comput. (2022), 18, 7093-7107 [DOI: 10.1021/acs.jctc.2c00882]
11. B. Hourahine, B. Aradi, V. Blum, F. Bonafé, A. Buccheri, C. Camacho, C. Cevallos, M. Y. Deshaye, T. Dumitrică, A. Dominguez, S. Ehlert, M. Elstner, T. van der Heide, J. Hermann, S. Irle, J. Jakowski, J. J. Kranz, C. Köhler, T. Kowalczyk, T. Kubař, I. S. Lee, V. Lutsker, R. J. Maurer, S. K. Min, I. Mitchell, C. Negre, T. A. Niehaus, A. M. N. Niklasson, A. J. Page, A. Pecchia, G. Penazzi, M. P. Persson, J. Řezáč, C. G. Sánchez, M. Sternberg, M. Stöhr, F. Stuckenberg, A. Tkatchenko, V. W.-z. Yu, T. Frauenheim , "*Erratum: "DFTB+, a software package for efficient approximate density functional theory based atomistic simulations*" [J. Chem. Phys. 152, 124101 (2020)], J. Chem. Phys. (2022)157, 039901 [DOI: 10.1063/5.0103026]
12. S. Garashchuk, J. Huang, B. G. Sumpter, J. Jakowski, *From Classical to Quantum Dynamics of Atomic and Ionic Species Interacting with Graphene and Its Analogue*", Theoretical and Computational Chemistry, (2022) 21, 61-86 [DOI: 10.1016/b978-0-12-819514-7.00001-4]
13. D. Lingerfelt, P. Ganesh, B.G. Sumpter, J. Jakowski*, From Ground to Excited Electronic State Dynamics of Electron and Ion Irradiated Graphene Nanomaterials*", Theoretical and Computational Chemistry, (2022) 21, 87-107, [DOI: 10.1016/b978-0-12-819514-7.00003-8]
14. Rajeev Kumar, Zening Liu, Brad Lokitz, Jihua Chen, Jan-Michael Carrillo, Jacek Jakowski, C. Patrick Collier, Scott Retterer & Rigoberto Advincula, *Harnessing autocatalytic reactions in polymerization and depolymerization*, MRS Communications (2021), [DOI: 10.1557/s43579-021-00061-9]
15. Kubra Yeter-Aydeniz, Bryan T. Gard, Jacek Jakowski, Swarnadeep Majumder, George S. Barron, George Siopsis, Travis Humble, and Raphael C. Pooser, *Benchmarking Quantum Chemistry Computations with Variational, Imaginary Time Evolution, and Krylov Space Solver Algorithm*s, Advanced Quantum Technologies (2021), [DOI: 10.1002/qute.202100012]
16. Lengwan Li, Jacek Jakowski, Changwoo Do, Kunlun Hong, *Deuteration and polymers: rich history with great potential,* Macromolecules, (2021), 54, 3555-3584 [DOI: 10.1021/acs.macromol.0c02284]
17. D. Lingerfelt, T. Yu, P. Ganesh, A. Yoshimura, J. Jakowski, B. G. Sumpter, *Nonadiabatic Effects on Defect Diffusion in Silicon-Doped Nanographenes*, Nano Lett. 21, 236–242 (2021) [DOI: 10.1021/acs.nanolett.0c03587]

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19. David B. Lingerfelt, Panchakepasan Ganesh, Jacek Jakowski, Bobby G Sumpter, *Understanding Beam Induced Electronic Excitations in Materials*, J, Chem. Theory and Comput. 16 (2), 1200-1214 (2020) [DOI: 10.1021/acs.jctc.9b00792]

20. Alexander J McCaskey, Zachary P Parks, Jacek Jakowski, Shirley V Moore, T Morris, Travis S Humble, Raphael C Pooser, *Quantum Chemistry as a Benchmark for Near-Term Quantum Computers,* Nature PJ-Quantum Information, 5:99 (2019) [DOI: 10.1038/s41534-019-0209-0]

21. David Lingerfelt, Panchakepasan Ganesh, Jacek Jakowski, Bobby G Sumpter, *Electronically Nonadiabatic Structural Transformations Promoted by Electron Beams*, Advanced Functional Materials, 1901901 (2019) [DOI: 10.1002/adfm.201901901]

22. Jordan A Hachtel, Jingsong Huang, Ilja Popovs, Santa Jansone-Popova, Jong K Keum, Jacek Jakowski, Tracy C Lovejoy, Niklas Dellby, Ondrej L Krivanek, Juan Carlos Idrobo *Damage-Free Nanoscale Isotopic Analysis of Biological Materials with Vibrational Electron Spectroscopy*, Microscopy and Microanalysis, (2019) 25, S2, 1088–1089, [DOI: 10.1017/S1431927619006172]

23. David Lingerfelt, Panchakepasan Ganesh, Jacek Jakowski, Bobby G Sumpter, *A TD-DFT Treatment of Electronic Excitations in the STEM Spanning Dipole and Impact Scattering Regimes*, Microscopy and Microanalysis, (2019) 25, S2, 2300,
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24. Jordan A. Hachtel, Jingsong Huang, Ilja Popovs, Santa Jansone-Popova, Jong K. Keum, Jacek Jakowski, Tracy C. Lovejoy, Niklas Dellby, Ondrej L. Krivanek, Juan Carlos Idrobo, *Identification of site-specific isotopic labels by vibrational spectroscopy in the electron microscope*, Science, 363, 525-528 (2019), [DOI: 10.1126/science.aav5845]

25. Tao Yu, Florence Fabunmi, Jingsong Huang, Bobby G Sumpter, Jacek Jakowski, *A Fast Scheme to Calculate Electronic Couplings between P3HT Polymer Units Using Diabatic Orbitals for Charge Transfer Dynamics Simulations*, J. Comp. Chem.40, 532-542 (2019), [DOI:10.1002/jcc.25749]

26. Dongsook Chang, Tianyu Li, Lengwan Li, Jacek Jakowski, Jingsong Huang, Jong Kahk Keum, Byeongdu Lee, Peter V. Bonnesen, Mi Zhou, Sophya Garashchuk, Bobby G. Sumpter, and Kunlun Hong *Selectively Deuterated Poly(ε-caprolactone)s: Synthesis and Isotope Effects on the Crystal Structures and Properties*, Macromolecules. [DOI: 10.1021/acs.macromol.8b01851]

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29. Zhiqi Hu, Jacek Jakowski, Chenyu Zheng, Christopher J. Collison, Joseph Strzalka, Bobby G. Sumpter, Rafael Verduzco, *An experimental and computational study of donor-linker-acceptor block copolymers for organic photovoltaics*", Journal of Polymer Science, Part B: Polymer Physics. 2018, 56, 1135–1143 (2018), [DOI: 10.1002/polb.24633]

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32. Niranji Thilini Ekanayake, Jingsong Huang, Jacek Jakowski, Bobby G. Sumpter, and Sophya Garashchuk, *Relevance of the Nuclear Quantum Effects on the Proton/Deuteron Transmission through Hexagonal Boron Nitride and Graphene Monolayers*, J. Phys. Chem. C. (2017), [DOI: 10.1021/acs.jpcc.7b08152]

33. Jacek Jakowski, Jingsong Huang, Sophya Garashchuk, Yingdong Luo, Kunlun Hong, Jong Keum, and Bobby G. Sumpter. *Deuteration as a Means to Tune Crystallinity of Conducting Polymers,* J. Phys. Chem. Lett. (2017), 8, pp 4333–4340, [DOI: 10.1021/acs.jpclett.7b01803]

34. Anton V. Ievlev, Jacek Jakowski, Mathew Burch, Vighter Iberi, Holland Hysmith, David C. Joy, Bobby G. Sumpter1, Alex Belianinov, Raymond R. Unocic, Olga S. Ovchinnikova, *Building with Ions: Towards Direct Write of Platinum Nanostructures using In-Situ Liquid Cell Helium Ion Microscopy*, Nanoscale (2017),9, 12949-12956 [DOI: 10.1039/C7NR04417H]

35. B.Yang, Chance C. Brown, Jingsong Huang, Liam Collins, Xiahan Sang, Raymond R. Unocic, Stephen Jesse, Sergei V. Kalinin, Alex Belianinov, Jacek Jakowski, David B. Geohegan, Bobby G. Sumpter, Kai Xiao, Olga S. Ovchinnikova, *Enhancing Ion Migration in Grain Boundaries of Hybrid Organic–Inorganic Perovskites by Chlorine*, Adv. Func. Mater. 1700749 (2017), [DOI: 10.1002/adfm.201700749]

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39. 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. 12 (9), 4487-450 (2016) [DOI: 10.1021/acs.jctc.6b00126]

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41. 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]

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43. 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]

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47. 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, 196-1210 (2013)[DOI: 10.1080/00268976.2013.783941]
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70. 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]

71. 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]

72. 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. Non-equilibrium Phenomena, Nonadiabatic Dynamics and Spectroscopy, *Modeling Electronic Structure, Dynamics and Properties of Conducting Polymers for Optoelectronic Applications* (invited talk), Telluride, Colorado, July 12-23, 2021
2. CECAM Workshop: Path Integral Quantum Mechanics: From the Basics to the Latest Developments, *Modeling Electronic Structure, Dynamics and Properties of Conducting Polymers for Optoelectronic Applications* (poster), hosted online, June 14-18, 2021
3. 2021 Spring ACS National Meeting, Symposium on Synergy between Quantum Computing and High-Performance Computing in Quantum Chemistry and Materials Science, *Quantum Chemistry Benchmark for Near-Term Quantum Computing* (invited talk), April 12, 2021
4. Clark Atlanta University, *Directing Transformations of Nanomaterials*, (invited seminar), Atlanta, GA, Nov. 5, 2019

5. CECAM Workshop: Thinking outside the box- beyond machine learning for quantum chemistry, *Directed Transformations of Nanomaterials* (invited talk) Bremen, Germany, Oct. 7-11, 2019,
6. Utah Workshop on Quantum Methods in Molecular and Solid State Theory, *Modeling electronic structure, dynamics and properties of conducting polymers for optoelectronic applications* (contributed talk), Park City, Utah, Sept. 22-27, 2019
7. Utah Workshop on Quantum Methods in Molecular and Solid State Theory, *Quantum Chemistry Benchmark for Near Time Quantum Computing*, (poster presentation), Park City, Utah, Sept 22-27, 2019
8. South Eastern Theoretical Chemistry Association 2019 Meeting (SETCA-2019), *Quantum Chemistry Benchmark for Near Time Quantum Computing*, (poster presentation), University of Tennessee, Knoxville, May 16-18, 2019,
9. APS March Meeting 2019, *Simulating Electron Beam – Materials Interactions with Real-Time Electron Dynamics* (contributed talk), Boston, MA, March 6, 2019
10. Workshop on Higher Category Approach to Certifiably Correct Quantum Information Processing Systems, *Quantum chemistry benchmark for quantum computing,* (invited talk) Beltsville, MD, Feb. 4, 2019
11. ORNL's CSMD/CSED Cross-Divisional Seminar Series, *Polymers Attack: Electronic Structure and Dynamics* (invited talk), ORNL, Oak Ridge, Nov, 07, 2018
12. Quantum Algorithms and Testbeds PI Meeting, *"Metrics and Benchmarks for Quantum Computing Quantum Testbed Pathfinder*", Travis Humble, Raphael Pooser, Kathleen Hamilton, Jacek Jakowski, Shirley Moore, Alex McCaskey, Megan Lilly, Titus Morris, Ryan Bennink, Sophia Economou, George Barron, Ken Brown, Natalie Brown (poster presentation), PI Meeting, Sponsored by the U.S. DOE, SciDAC Division, Oak Ridge TN, September 18 - 19, 2018
13. MRS meeting, *Deuteration as a Means to Tune Properties of Conducting Polymers* (contributed talk) Phoenix, AZ, April 2-6, 2018
14. Sanibel Symposium, "*The effect of isotope substitution on stability and dynamics of polymers*" (poster), St. Simons Island, GA, Feb. 12-18, 2018
15. 2016 South Eastern Regional Meeting of American Chemical Society (2016 SERMACS), *Isotope substitution, electronic structure and dynamics in conducting polymers,* Jacek Jakowski, October 20, 2016 (invited talk).
16. *251th National ACS Meeting,* San Diego, "*Rupture of a graphene membrane under an electric field using DFTB*", Krystle Reiss, Jacek Jakowski, James Mazzuca (poster, Reiss presented) 03/16/2016
17. *251th National ACS Meeting,* San Diego, "Density functional tight binding with ScaLAPACK for efficient electronic structure calculations", Jacob Blazejewski, Jacek Jakowski, James Mazzuca (poster, Blazejewski presented), 03/16/2016
18. Quantum Chemistry Laboratory seminar, *Crossing scales: from electron dynamics to quantum protons in nanoscale systems* (seminar), Dept. of Chemistry, University of Warsaw, Poland, October 22, 2015
19. *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 Nanomaterial*".
20. Wiley Seminar, *Modeling multiphysics processes of nano-scale systems with tight-binding DFT methods* (seminar), PNNL, Richland, WA, Sept. 25, 2015
21. *Beyond Exascale: Qubits for Quantum Computing* Workshop, "*Tight-Binding Density Functional Theory (DFT) Methods for Understanding Dynamics in Nanostructures"* (invited talk), Oak Ridge, TN, Aug 20-21, 2015,

22. *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)
23. 248th National ACS Meeting*,* San Francisco, *"Quantum reaction dynamics of nanoscale materials*", August 14, 2014 (contributing talk)
24. 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)
25. 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)
26. *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.*
27. 2013 Telluride Science Research Center Conference on Advances In Photoreactions: When SpinOrbit Coupling, Optical Excitation, and Motion of Nuclei are of Equal Importance, Telluride, CO, June 22-25, 2013, *"Modeling Materials at the Nanoscale"* (invited lecture)
28. 53rd Sanibel Symposium, St. Simons Island, GA, Feb. 17-22, 2013, "*Modeling Materials at the Nanoscale- Quantum Dynamical Perspective*" (invited plenary lecture)
29. XSEDE -ECSS symposium, *Development of New Quantum Chemical Molecular Dynamics for Materials Science Modeling* , 04/16/2013
30. Jacek Jakowski, "*Computational Advanced Materials Endstation on HPC architectures", at the "Tennessee CyberInfrastructure Symposium*" 04/04/2013, TSU, Nashville, (invited talk)
31. NCCS/ORNL seminar, *Modeling Advanced Materials. EPSCoR Desktop to Petascale Ecosystem* (seminar), October 31, 2013,
32. "*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)
33. 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)
34. 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)
35. "*Electron Transfer and Energy Transfer in Carbon Materials*" at the 14th International Congress of Quantum Chemistry, Boulder, CO, June 25-30, 2012 (poster)
36. "*Real time simulations of electron transfer and energy transfer in carbon materials*", Clemson University, April 8, 2012 (seminar)
37. "*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)
38. "*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)
39. 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)

40. "*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)
41. "*Electronic structure on GPU*" at the "HPC in Chemistry" workshop, Knoxville, TN, Aug 8, 2011 (talk)
42. "*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)
43. "*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)
44. "*Liouville von Neumann Molecular Dynamics*" at the GRS/JICS workshop on Large-Scale Computer Simulation. Aachen / Jülich, Germany, March 9-11, 2011 (invited talk)
45. "*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)
46. "*Liouville-von Neumann dynamics on GPU*", at the 240th National Meeting of the American Chemical Society, Boston, MA, August 22, 2010 (talk)