Alexander Yu. Sokolov

Curriculum Vitae

Contact Information

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Professional Experience

Current 8/2017	*Assistant Professor* **The Ohio State University**, Columbus, OH (USA) Department of Chemistry & Biochemistry
7/2016 – 8/2017	*Postdoctoral Scholar* **California Institute of Technology**, Pasadena, CA (USA) Advisor: Professor Garnet K.-L. Chan
8/2014 – 6/2016	*Postdoctoral Research Associate* **Princeton University**, Princeton, NJ (USA) Advisor: Professor Garnet K.-L. Chan

Education

2009 – 2014	*Doctor of Philosophy* **University of Georgia**, Center for Computational Quantum Chemistry, Athens, GA (USA) Advisor: Professor Henry F. Schaefer III Thesis: "Development of density cumulant functional theory"
2004 – 2009	*Specialist Degree (M.S.)* **St. Petersburg State University**, St. Petersburg (Russia) *Diploma with Distinction* | Major: Chemistry Advisor: Professor Olga V. Sizova Thesis: "Valence structure analysis of heavy transition metal complexes with electronic configurations d^6, d^7, d^8, and d^{10}"

Academic Awards

2016	American Chemical Society Physical Chemistry Division Postdoctoral Award
2015	IBM-Löwdin Award for Postdoctoral Associates, 55^{th} Sanibel Symposium, St. Simons' Island, GA (USA)
2014	Martin Reynolds Smith Award, University of Georgia, Athens, GA (USA)
2013	Dissertation Completion Award, University of Georgia, Athens, GA (USA)
2013	Best Graduate Student Poster Award, 53^{rd} Sanibel Symposium, St. Simons' Island, GA (USA)
2012	James L. Carmon Award, University of Georgia, Athens, GA (USA)
2009	Best Alumnus of St. Petersburg 2009 Award, St. Petersburg (Russia)

Fellowships

2009 – 2014	Charles Coulson Fellowship, Center for Computational Quantum Chemistry, Athens, GA (USA)
2008 – 2009	Special Scholarship of the Government of Russian Federation (Russia)
5 – 8/2008	Summer Fellowship, Center for Computational Quantum Chemistry, Athens, GA (USA)
2004 – 2009	Full Scholarship, St. Petersburg State University (Russia)

Teaching Experience

2018	Advanced Quantum Mechanics and Spectroscopy (CHEM 7520), *Instructor*, OSU
2011 – 2014	Advanced Quantum Chemistry (CHEM 8950), *Teaching Assistant*, UGA
2011, 2012	Summer Undergraduate Fellowship Program, *Instructor and Mentor*, Center for Computational Quantum Chemistry, UGA
2010 – 2011	General Chemistry Laboratory I and II, *Teaching Assistant*, UGA
2008	General and Inorganic Chemistry, *Teaching Assistant*, St. Petersburg State University (Russia)

Invited Talks

08/2019	Symposium in Honor of Henry F. Schaefer, 258^{th} ACS National Meeting, San Diego, CA (USA)
03/2019	Symposium "Quantum Mechanics: Strong Correlation", 257^{th} ACS National Meeting, Orlando, FL (USA)
11/2018	Psi4 Annual Developer's Conference (PsiCon), Atlanta, GA (USA)
06/2018	50^{th} Midwest Theoretical Chemistry Conference, Chicago, IL (USA)
07/2017	Workshop "New Developments in Coupled-Cluster Theory", Telluride, CO (USA)
05/2017	Symposium "Electronic Structure Theory", 100^{th} Canadian Chemistry Conference, Toronto (Canada)
04/2017	Symposium "Strong Electron Correlation & Nonadiabatic Dynamics", 253^{rd} ACS National Meeting, San Francisco, CA (USA)
08/2016	Symposium "Metal & Semiconductor Nanoclusters with Atomic Precision: Fundamentals & Applications", *ACS Physical Chemistry Division Postdoctoral Award Talk*, 252^{nd} ACS National Meeting, Philadelphia, PA (USA)
06/2016	8^{th} Molecular Quantum Mechanics (MQM) Congress, Uppsala University, Uppsala (Sweden)
03/2016	Symposium "Towards Predictive Calculations in Strongly Correlated Molecules and Materials", 251^{st} ACS National Meeting, San Diego, CA (USA)
08/2015	Workshop on Quantum Marginals and Numerical Ranges, University of Guelph, Guelph (Canada)
05/2014	Annual Meeting of the Southeast Theoretical Chemistry Association (SETCA 2014), Atlanta, GA (USA)
09/2013	Quantum Mechanics in Many Dimensions, 246^{th} ACS National Meeting, Indianapolis, IN (USA)
06/2013	Max Planck Institut für Chemische Energiekonversion, Mülheim (Germany)
06/2013	Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, Bochum (Germany)

Scholarly Activities

Reviewer for the following journals:

- Journal of Chemical Theory and Computation
- Journal of Chemical Physics
- Physical Chemistry Chemical Physics
- International Journal of Quantum Chemistry
- Theoretical Chemistry Accounts
- New Journal of Chemistry
- Acta Physica Polonica A

Reviewer for the funding agencies and computing facilities:

- National Science Foundation
- American Chemical Society Petroleum Research Fund
- Swiss National Science Foundation
- The Ohio Supercomputer Center

Professional Societies

- American Chemical Society

Publications

[1] **A. Yu. Sokolov**. "Multi-reference algebraic diagrammatic construction theory for excited states: General formulation and first-order implementation." *J. Chem. Phys.* **149**, 204113 (2018). (Highlight: **JCP Editors' Pick article**).

[2] A. V. Copan and **A. Yu. Sokolov**. "Linear-response density cumulant theory for excited electronic states." *J. Chem. Theory Comput.* **14**, 4097–4108 (2018).

[3] **A. Yu. Sokolov**, S. Guo, E. Ronca, and G. K.-L. Chan. "Time-dependent N-electron valence perturbation theory with matrix product state reference wavefunctions for large active spaces and basis sets: Applications to the chromium dimer and all-trans polyenes." *J. Chem. Phys.* **146**, 244102 (2017).

[4] R. M. Parrish, L. A. Burns, D. G. A. Smith, A. C. Simmonett, A. E. DePrince, E. G. Hohenstein, U. Bozkaya, **A. Yu. Sokolov**, R. Di Remigio, R. M. Richard, J. F. Gonthier, A. M. James, H. R. McAlexander, A. Kumar, M. Saitow, X. Wang, B. P. Pritchard, P. Verma, H. F. Schaefer, K. Patkowski, R. A. King, E. F. Valeev, F. A. Evangelista, J. M. Turney, T. D. Crawford, and C. D.

Sherrill. "Psi4 1.1: An Open-Source Electronic Structure Program Emphasizing Automation, Advanced Libraries, and Interoperability." *J. Chem. Theory Comput.* **13**, 3185–3197 (2017).

[5] X. Wang, **A. Yu. Sokolov**, J. M. Turney, and H. F. Schaefer. "Spin-adapted formulation and implementation of density cumulant functional theory with density-fitting approximation: Application to transition metal compounds." *J. Chem. Theory Comput.* **12**, 4833–4842 (2016).

[6] **A. Yu. Sokolov** and G. K.-L. Chan. "A time-dependent formulation of multi-reference perturbation theory." *J. Chem. Phys.* **144**, 064102 (2016). (Highlight: **JCP 2016 Editors' Choice article**).

[7] J. W. Mullinax, **A. Yu. Sokolov**, and H. F. Schaefer. "Can density cumulant functional theory describe static correlation effects?" *J. Chem. Theory Comput.* **11**, 2487–2495 (2015).

[8] **A. Yu. Sokolov** and G. K.-L. Chan. "A transformed framework for dynamic correlation in multireference problems." *J. Chem. Phys.* **142**, 124107 (2015).

[9] **A. Yu. Sokolov**, H. F. Schaefer, and W. Kutzelnigg. "Density cumulant functional theory from a unitary transformation: N-representability, three-particle correlation effects, and application to O_4^+." *J. Chem. Phys.* **141**, 074111 (2014).

[10] J. W. Mullinax, **A. Yu. Sokolov**, and H. F. Schaefer. "Conical intersections and low-lying electronic states of tetrafluoroethylene." *ChemPhysChem* **15**, 2359–2366 (2014).

[11] A. V. Copan, **A. Yu. Sokolov**, and H. F. Schaefer. "Benchmark study of density cumulant functional theory: thermochemistry and kinetics." *J. Chem. Theory Comput.* **10**, 2389–2398 (2014).

[12] **A. Yu. Sokolov** and H. F. Schaefer. "Orbital-optimized density cumulant functional theory." *J. Chem. Phys.* **139**, 204110 (2013).

[13] **A. Yu. Sokolov**, D. B. Magers, J. I. Wu, W. D. Allen, P. v. R. Schleyer, and H. F. Schaefer. "Free cyclooctatetraene dianion: planarity, aromaticity, and theoretical challenges." *J. Chem. Theory Comput.* **9**, 4436–4443 (2013).

[14] Y. Qiu, **A. Yu. Sokolov**, Y. Yamaguchi, and H. F. Schaefer. "$BeCH_2$: the simplest metal carbene. High levels of theory." *J. Phys. Chem. A* **117**, 9266–9273 (2013).

[15] S. Vogt-Geisse, **A. Yu. Sokolov**, S. R. McNew, Y. Yamaguchi, and H. F. Schaefer. "Structures and transition states of Ge_2CH_2." *J. Phys. Chem. A* **117**, 5765–5774 (2013).

[16] **A. Yu. Sokolov**, A. C. Simmonett, and H. F. Schaefer, III. "Density cumulant functional theory: the DC-12 method, an improved description of the one-particle density matrix." *J. Chem. Phys.* **138**, 024107 (2013).

[17] **A. Yu. Sokolov**, S. Mittal, A. C. Simmonett, and H. F. Schaefer III. "Characterization of the t-butyl radical and its elusive anion." *J. Chem. Theory Comput.* **8**, 4323–4329 (2012).

[18] **A. Yu. Sokolov**, J. J. Wilke, A. C. Simmonett, and H. F. Schaefer III. "Analytic gradients for density cumulant functional theory: the DCFT-06 model." *J. Chem. Phys.* **137**, 054105 (2012).

[19] **A. Yu. Sokolov** and H. F. Schaefer III. "Ground and excited state properties of photoactive platinum(IV) diazido complexes: theoretical considerations." *Dalton Trans.* **40**, 7571–7582 (2011).

[20] **A. Yu. Sokolov** and H. F. Schaefer III. "Coordination properties of bridging diazene ligands in unusual diiron complexes." *Organometallics* **29**, 3271–3280 (2010).

[21] **A. Yu. Sokolov** and O. V. Sizova. "Quantum-chemical study of trans-influence in gold(I) linear complexes." *Russ. J. Gen. Chem.* **80**, 1223–1231 (2010).

[22] V. V. Pakal'nis, **A. Yu. Sokolov**, A. A. Slisenko, M. E. Borovitov, S. P. Tunik, and O. V. Sizova. "Synthesis and spectral characteristics of a novel heterometallic binuclear complex on the basis of 3,6-bis(2-pyridyl)-1,2,4,5-tetrazine." *Russ. J. Gen. Chem.* **79**, 980–984 (2009).

[23] O. V. Sizova, L. V. Skripnikov, **A. Yu. Sokolov**, and V. V. Sizov. "Atomic-orbital-symmetry based σ-, π-, and δ-decomposition analysis of bond orders." *Int. J. Quant. Chem.* **109**, 2581–2590 (2009).

[24] O. V. Sizova, L. V. Skripnikov, and **A. Yu. Sokolov**. "Calculation of σ-, π-, and δ-components of quantum-chemical bond orders." *Russ. J. Gen. Chem.* **78**, 2146–2147 (2008).

[25] O. V. Sizova, L. V. Skripnikov, and **A. Yu. Sokolov**. "Symmetry decomposition of quantum-chemical bond orders." *J. Mol. Struct. (THEOCHEM)* **870**, 1–9 (2008).

[26] **A. Yu. Sokolov**, N. J. Stibrich, and H. F. Schaefer III. "BO_3 molecular structures: examples of the importance of electron correlation." *Coll. Czech. Chem. Commun.* **73**, 1495–1508 (2008).

[27] O. V. Sizova, **A. Yu. Sokolov**, and L. V. Skripnikov. "Quantum-chemical study of donor-acceptor interactions in chelate dicarbonyl complexes of rhodium(I)." *Russ. J. Coord. Chem.* **33**, 800–808 (2007).

[28] O. V. Sizova, **A. Yu. Sokolov**, L. V. Skripnikov, and V. I. Baranovski. "Quantum chemical study of the bond orders in the ruthenium, diruthenium and dirhodium nitrosyl complexes." *Polyhedron* **26**, 4680–4690 (2007).

[29] O. V. Sizova, L. V. Skripnikov, **A. Yu. Sokolov**, and N. V. Ivanova. "Rhodium and ruthenium tetracarboxylate nitrosyl complexes: electronic structure and metal-metal bond." *Russ. J. Coord. Chem.* **33**, 588–593 (2007).

[30] O. V. Sizova, L. V. Skripnikov, **A. Yu. Sokolov**, and O. O. Lyubimova. "Features of the electronic structure of ruthenium tetracarboxylates with axially coordinated nitric oxide (II)." *J. Struct. Chem.* **48**, 28–36 (2007).