

Published Journal Articles with Graduate Student Co-authors

Organized by Faculty Mentor
Department of Chemistry and Biochemistry
Publication dates: January, 2011 - June, 2016

Antony, Edwin

Journal Article, Academic Journal (Published)

Lytle, A., Origanti, S. S., Qiu, Y., Vongermeten, J., Myong, S., Antony, E. (2014). Context-Dependent Remodeling of Rad51-DNA Complexes by Srs2 Is Mediated by a Specific Protein-Protein Interaction. *Journal of Molecular Biology*, 1(426), 1883-1897.
<http://www.sciencedirect.com/science/article/pii/S0022283614000965>

Journal Article, Professional Journal (Published)

Duval, S., Danyal, K., Shaw, S., Lytle, A. K., Dean, D. R., Hoffman, B. M., Antony, E., Seefeldt, L. (2013). Electron transfer precedes ATP hydrolysis during nitrogenase catalysis. *Proc. Natl. Acad. Sci. USA*, 110, 16414-16419.

Berreau, Lisa M.

Journal Article, Academic Journal (Published)

Anderson, S. N., Richards, J. M., Esquer, H. J., Benninghoff, A., Arif, A. M., Berreau, L. (2015). A New Structurally-Tunable 3-Hydroxyflavone Motif for Visible Light-induced CO-releasing Molecules. *ChemistryOpen*, 4(5), 590-594.
onlinelibrary.wiley.com/doi/10.1002/open.201500167/abstract

Journal Article, Academic Journal (Published)

Berreau, L., Allpress, C. J., Milaczewska, A., Borowski, T., Bennett, J. R., Tierney, D. L., Arif, A. M. (2014). Halide-promoted Dioxygenolysis of a Carbon-carbon bond by a Copper(II) Diketonate Complex. *J. Am. Chem. Soc.*, 136, 7821+7824.

Journal Article, Academic Journal (Published)

Anderson, S. N., Noble, M., Grubel, K., Marshall, B., Arif, A. M., Berreau, L. (2014). Influence of Supporting Ligand Microenvironment on the Aqueous Stability and Visible Light Induced CO Release Reactivity of Zinc Flavonolate Species. *Journal of Coordination Chemistry*, 67, 4061-4075.

Journal Article, Academic Journal (Published)

Saraf, S. L., Fish, T., Benninghoff, A., Buelt, A., Smith, R. C., Berreau, L. (2014). Photochemical Reactivity of Ru(II)(n6-p-cymene) Flavonolate Complexes. *American Chemical Society*, 33(22), 6341-6351. pubs.acs.org/doi/abs/10.1021/om5006337

Journal Article, Academic Journal (Published)

Allpress, C. J., Berreau, L. (2013). Oxidative Aliphatic Carbon-carbon Bond Cleavage Reactions. *Coord. Chem. Rev.*, 257, 3005-3029.

Journal Article, Academic Journal (Published)

Grubel, K., Saraf, S. L., Anderson, S. N., Laughlin, B. J., Smith, R. C., Arif, A. M., Berreau, L. (2013). Synthesis, Characterization, and Photoinduced CO-release Reactivity of a Pb(II) Flavonolate Complex; Comparisons to Group 12 Analogs. *Inorg. Chim. Acta*, 407, 91-97.

Journal Article, Professional Journal (Published)

Allpress, C. J., Grubel, K., Szajna-Fuller, E., Arif, A. M., Berreau, L. (2013). Regioselective Aliphatic Carbon-carbon Bond Cleavage by a Model System of Relevance to Iron-containing Acireductone Dioxygenase (Fe-ARD'). *J. Am. Chem. Soc.*, 135(2), 659-668.

Journal Article, Professional Journal (Published)

Allred, R. A., Bebout, D. C., ARif, A. M., Berreau, L. (2012). Mercury Coordination Chemistry of a Nitrogen/Sulfur Ligand Having an Internal Hydrogen Bond Donor: Generation of a Thioether-coordinated Dimercurous Complex. *Main Group Chemistry*, 11, 53-67.

Journal Article, Professional Journal (Published)

Grubel, K., Marts, A. R., Greer, S. M., Tierney, D. L., Allpress, C. J., Anderson, S. N., Laughlin, B. J., Smith, R. C., Arif, A. M., Berreau, L. (2012). Photoinitiated Dioxygenase-type Reactivity of Open-shell 3d Divalent Metal Flavonolate Complexes. *European Journal of Inorganic Chemistry*, 4750-4757.

Journal Article, Academic Journal (Published)

Grubel, K., Ingle, G. K., Fuller, A. L., Arif, A. M., Berreau, L. (2011). Influence of Water on the Formation of O₂-reactive Divalent Metal Enolate Complexes of Relevance to Acireductone Dioxygenases. *Dalton Transactions*, 40, 10609-10620.

Journal Article, Academic Journal (Published)

Berreau, L., Borowski, T., Grubel, K., Allpress, C. J., Wikstrom, J. P., Germain, M. E., Rybak-Akimova, E. V., Tierney, D. L. (2011). Mechanistic Studies of the O₂-dependent Aliphatic Carbon-carbon Bond Cleavage Reaction of a Nickel Enolate Complex. *Inorganic Chemistry*, 50, 1047-1057.

Journal Article, Academic Journal (Published)

Grubel, K., Laughlin, B. J., Maltais, T. R., Smith, R. C., Arif, A. M., Berreau, L. (2011). Photochemically-induced Dioxygenase-type CO-release Reactivity of Group 12 Metal Flavonolate Complexes. *Chemical Communications*, 47, 10431-10433.

Journal Article, Academic Journal (Published)

Allpress, C. J., Arif, A. M., Houghton, D. T., Berreau, L. (2011). Photochemically-induced Oxidative Carbon-carbon Bond Cleavage Reactivity in Chlorodiketonate Ni(II) Complexes. *Chemistry - A European Journal*, 17, 14962-14973.

Journal Article, Academic Journal (Accepted)

Allpress, C. J., Berreau, L. (2014). A Nickel-containing Model System of Acireductone Dioxygenases that Utilizes a C(1)-H Acireductone Substrate. *Eur. J. Inorg. Chem.*(27), 4642-4649.

Journal Article, Professional Journal (Submitted)

Anderson, S. N., Berreau, L. (2016). A Heterogeneous In Situ PhotoCORM for Aerobic Palladium-catalyzed Carbonylation. *Chemical Communications*.

Journal Article, Academic Journal (Submitted)

Saraf, S. L., Milaczewska, A., Borowski, T., James, C. D., Tierney, D. L., Popova, M., Arif, A. M., Berreau, L. (2016). Anion Effects in Oxidative Aliphatic Carbon-carbon Bond Cleavage Reactions of Cu(II) Chlorodiketonate Complexes. *Inorganic Chemistry*.

Journal Article, Academic Journal (Submitted)

Anderson, S. N., Berreau, L. (2016). Solution or solid - it doesn't matter: Dioxygenase-type visible light induced CO release chemistry of zinc flavonolato complexes. *Dalton Transactions*.

Bialkowski, Stephen E.

Journal Article, Academic Journal (Published)

Dada, O. O., Bialkowski, S. E. (2011). A Compact Pulsed Infrared Laser Excited Photothermal Deflection Spectrometer. *Applied Spectroscopy*, 65, 201.

Boldyrev, Alexander I.

Journal Article, Academic Journal (Published)

Zhou, X.-F., Oganov, A. R., Wang, Z., Popov, I. A., Boldyrev, A. I., Wang, H.-T. (2016). Two-dimensional magnetic boron. *Physivcal Review B*, 93, 085406 (number of the article).

Journal Article, Academic Journal (Published)

Ivanov, A. S., Kar, T., Boldyrev, A. I. (2016). Nanoscale Stabilization of Zintl Compounds: 1D Ionic Li-P Double Helix Confined Inside a Carbon Nanotube. *Nanoscale*, 8, 3454-3460.

Journal Article, Academic Journal (Published)

Yu, X., Oganov, A. R., Popov, I. A., Qian, G., Boldyrev, A. I. (2016). Antiferromagnetic Stabilization in the Ti8O12 Cluster. *Angewandte Chemie International Edition*, 55(5), 1699-1703.

Journal Article, Academic Journal (Published)

Yu, X., Oganov, A. R., Popov, I. A., Boldyrev, A. I. (2016). d-AO Spherical Aromaticity in Ce6O8. *Journal Computational Chemistry*, 37, 103-109.

Journal Article, Academic Journal (Published)

Nizovtsev, A. S., Ivanov, A. S., Boldyrev, A. I., Konchenko, S. N. (2015). Li4E8 (E = P, As, Sb, Bi) Clusters: The Quest for Realgar-Type [E8]4- Zintl Anions. *European Journal of Inorganic Chemistry*, 2015(35), 5801–5807.

Journal Article, Academic Journal (Published)

Ivanov, A. S., Zhang, X., Wang, H., Boldyrev, A. I., Gantefoer, G. F., Bowen, K. H., Černušák, I. (2015). Anion Photoelectron Spectroscopy and CASSCF/CASPT2/RASSI Study of Lan- (n=1, 3-7). *Journal of Physical Chemistry A*, 119, 11293-11303.

Journal Article, Academic Journal (Published)

Popov, I. A., Jian, T., Lopez, G. V., Boldyrev, A. I., Wang, L.-S. (2015). Cobalt-centred boron molecular drums with the highest coordination number in the CoB16- cluster. *Nature Communication*, 6, 8654.

Journal Article, Academic Journal (Published)

Yang, L.-M., Popov, I. A., Frauenheim, T., Boldyrev, A. I., Heine, T., Bacic, V., Ganz, E. (2015). Revealing Unusual Chemical Bonding in Planar Hyper-Coordinate Ni2Ge and Quasi-Planar Ni2Si Two-Dimensional Crystals. *Physical Chemistry Chemical Physics*, 17, 26043-26048.

Journal Article, Academic Journal (Published)

Popov, I. A., Zhang, X., Eichhorn, B. W., Boldyrev, A. I., Bowen, K. H. (2015). Aluminum Chain in Li2Al3H8- as Suggested by Photoelectron Spectroscopy and ab initio Calculations. *Physical Chemistry Chemical Physics*, 17, 26079-26083.

Journal Article, Academic Journal (Published)

Dolyniuk, J.-A., He, H., Ivanov, A. S., Boldyrev, A. I., Bobev, S., Kovnir, K. (2015). Ba and Sr Binary Phosphides: Synthesis, Crystal Structures, and Bonding Analysis. *Inorganic Chemistry*, 54(17), 8608-8616.

Journal Article, Academic Journal (Published)

Yang, L.-M., Popov, I. A., Boldyrev, A. I., Heine, T., Frauenheim, T., Granz, E. (2015). Post-anti-van't Hoff-Le Bel Motif in Atomically Thin Germanium-Copper Alloy Film. *Physical Chemistry Chemical Physics*, 17, 17545-17551.

Journal Article, Academic Journal (Published)

Ivanov, A. S., Miller, E., Boldyrev, A. I., Kameoka, Y., Sato, T., Tanaka, K. (2015). Pseudo Jahn-Teller Origin of Buckling Distortions in Two-Dimensional Triazine-Based Graphitic Carbon Nitride (g-C₃N₄) Sheets. *The Journal of Physical Chemistry C*, 119(21), 12008-12015.

Journal Article, Academic Journal (Published)

Gish, J. T., Popov, I. A., Boldyrev, A. I. (2015). Homocatenation of Aluminum: Alkane-like Structures of Li₂Al₂H₆ and Li₃Al₃H₈. *Chemistry - European Journal*, 21(14), 5307-5310.

Journal Article, Academic Journal (Published)

Yang, L.-M., Basic, V., Popov, I. A., Boldyrev, A. I., Heine, T., Frauenheim, T., Ganz, E. (2015). Two-dimensional Cu₂Si Monolayer with Planar Hexacoordinate Copper and Silicon Bonding. *Journal of The American Chemical Society*, 137(7), 2757-2762.

Journal Article, Academic Journal (Published)

Popov, I. A., Averkiev, B. B., Starikova, A. A., Boldyrev, A. I., Minyev, R. M., Minkin, V. I. (2014). Assessing the Viability of Extended Nonmetal Atom Chains in MnF_{4n+2} (M=S and Se). *Angewandte Chemie International Edition*, 54(5), 1476-1480.

Journal Article, Academic Journal (Published)

Minyayev, R. M., Popov, I. A., Koval, V. V., Boldyrev, A. I., Minkin, V. I. (2014). Supertetrahedral B₈₀H₂₀, C₈₀H₂₀, and Al₈₀H₂₀ Analogs of Dodecahedrane and their Substituted Molecules. *Structural Chemistry*, 26(1), 223-229.

Journal Article, Academic Journal (Published)

Ivanov, A. S. (2014). Paper Deciphering aromaticity in porphyrinoids via adaptive natural density partitioning. *Organic & Biomolecular Chemistry*, 12, 6145-6150.
<http://pubs.rsc.org/en/journals/journalissues/ob#!recentarticles&all>

Journal Article, Academic Journal (Published)

Ivanov, A., Boldyrev, A. I., Frenking, G. (2014). Inorganic Double-Helix Nanotoroid of Simple Lithium-Phosphorus Species. *Chem. Eur. J.*, 20, 2431-2435.

Journal Article, Academic Journal (Published)

Popov, I., Piazza, Z., Li, W.-L., Wang, L.-S., Boldyrev, A. I. (2014). Complexes between planar boron clusters and transition metals: a photoelectron spectroscopy and ab initio study of CoB₁₂- and RhB₁₂-. *J. Phys. Chem. A*.

Journal Article, Academic Journal (Published)

Ivanov, A., Frenking, G., Boldyrev, A. I. (2014). Stabilization of Cl-Cl- Anion Pair in the Gas Phase: Ab Initio Microsolvation Study. *J. Phys. Chem. A*.

Journal Article, Academic Journal (Published)

Popov, I., Piazza, Z., Li, W.-L., Wang, L.-S., Boldyrev, A. I. (2013). A combined photoelectron spectroscopy and ab initio study of the quasi-planar B₂₄- cluster. *J. Chem. Phys.*, 139, 114307.

Journal Article, Academic Journal (Published)

Popov, I., Popov, V., Bozhenko, K., Cernusak, I., Boldyrev, A. I. (2013). Structural changes in the series of boron-carbon mixed clusters C_xB_{10-x} ($x = 3-10$) upon substitution of boron by carbon. *J. Chem. Phys.*, 139, 144307.

Journal Article, Academic Journal (Published)

Li, W.-L., Ivanov, A., Federic, J., Romanescu, C., Cernusak, I., Boldyrev, A. I., Wang, L.-S. (2013). On the way to the highest coordination number in the planar metal-centered aromatic $Ta@B_{10}$ - cluster: Evolution of the Structures of TaB_n - ($n=3-8$). *J. Chem. Phys.*, 139, 104312.

Journal Article, Academic Journal (Published)

Romanescu, C., Galeev, T., Li, W.-L., Boldyrev, A. I., Wang, L.-S. (2013). Geometric and electronic factors in the rational design of transition-metal-centered boron molecular wheels. *J. Chem. Phys.*, 138, 134315.

Journal Article, Academic Journal (Published)

Popov, I., Li, Y., Chen, Z., Boldyrev, A. I. (2013). "Benzation" of graphene upon addition of monovalent chemical species. *Phys. Chem. Chem. Phys.*, 15, 6842-6848.

Journal Article, Academic Journal (Published)

Galeev, T., Dunnington, B., Schmidt, J.R., Boldyrev, A. I. (2013). Solid State Adaptive Natural Density Partitioning: A Tool for Deciphering Multi-center Bonding in Periodic Systems. *Phys. Chem. Chem. Phys.*, 15, 5022-5029.

Journal Article, Academic Journal (Published)

Olson, J., Boldyrev, A. I. (2013). Planar to 3D Transition in the B_6Hy Anions. *J. Phys. Chem. A*, 117, 1614-1620.

Journal Article, Academic Journal (Published)

Popov, I., Boldyrev, A. I. (2013). Computational Probing of All-Boron $Li_2nB_{2n}H_{2n+2}$ Polyenes. *Comp. Theor. Chem*, 1004, 5-11.

Journal Article, Academic Journal (Published)

Romanescu, C., Galeev, T. R., Sergeeva, A. P., Li, W.-L., Wang, L.-S., Boldyrev, A. I. (2012). Experimental and Computational Evidence of Octa- and Nona-Coordinated Planar Iron-Doped Boron Clusters: $Fe@B_8$ - and $Fe@B_9$ -. *Journal of Organometallic Chemistry*, 721-722, 148-154. <http://www.sciencedirect.com/science/article/pii/S0022328X12005050>

Journal Article, Academic Journal (Published)

Ivanov, A., Boldyrev, A. I. (2012). Reliable Predictions of Unusual Molecules. *Physical Chemistry Chemical Physics*, 14, 15943-15952. <http://pubs.rsc.org/en/content/articlelanding/2012/cp/c2cp42877f>

Journal Article, Academic Journal (Published)

Sergeeva, A. P., Piazza, Z. A., Romanescu, C., Li, W.-L., Boldyrev, A. I., Wang, L.-S. (2012). B_{22} - and B_{23} -: All-Boron Analogues of Anthracene and Phenanthrene. *Journal of The American Chemical Society*, 134(43), 18065-18073.

Journal Article, Academic Journal (Published)

Ivanov, A. S., Boldyrev, A. I. (2012). $Si_6-nC_nH_6$ ($n = 0-6$) Series: When Do Silabenzenes Become Planar and Global Minima? *The Journal of Physical Chemistry A*, 116(38), 9591-9598. <http://pubs.acs.org/doi/abs/10.1021/jp307722q?journalCode=jpcafh>

Journal Article, Academic Journal (Published)

Ivanov, A. S., Bozhenko, K. V., Boldyrev, A. I. (2012). On the Suppression Mechanism of the Pseudo-Jahn-Teller Effect in Middle E6 (E = P, As, Sb) Rings of Triple-Decker Sandwich Complexes. *Inorganic Chemistry*, 51(16), 8868–8872.
<http://pubs.acs.org/doi/abs/10.1021/ic300786w?journalCode=inocaj>

Journal Article, Academic Journal (Published)

Ivanov, A. S., Morris, A. J., Bozhenko, K. V., Pickard, C. J., Boldyrev, A. I. (2012). Inorganic Double-Helix Structures of Unusually Simple Li-P Species. *ngewandte Chemie International Edition*, 51(33), 8330–8333.
<http://onlinelibrary.wiley.com/doi/10.1002/anie.201201843/abstract>

Journal Article, Academic Journal (Published)

Boldyrev, A. I., Osorio, E., Olson, J. K., Tiznado, W. (2012). Analysis of Why Boron Avoids sp² Hybridization and Classical Structures in the BnHn+2 Series. *Chemistry - A European Journal*, 18(31), 9677–9681.
<http://onlinelibrary.wiley.com/doi/10.1002/chem.201200506/abstract>

Journal Article, Academic Journal (Published)

Popov, I. A., Boldyrev, A. I. (2012). Chemical Bonding in Coronene, Isocoronene, and Circumcoronene. *European Journal of Organic Chemistry*, 2012(18), 3485–3491.
<http://onlinelibrary.wiley.com/doi/10.1002/ejoc.201200256/abstract>

Journal Article, Academic Journal (Published)

Piazza, Z. A., Li, W.-L., Romanescu, C., Sergeeva, A. P., Wang, L.-S., Boldyrev, A. I. (2012). A photoelectron spectroscopy and ab initio study of B₂₁⁻: Negatively charged boron clusters continue to be planar at 21. *The Journal of Chemical Physics*, 136, 104310.
<http://dx.doi.org/10.1063/1.3692967>

Journal Article, Academic Journal (Published)

Popov, I. A., Bozhenko, K. V., Boldyrev, A. I. (2012). Is Graphene Aromatic? *Nano Research*, 5(2), 117-123. <http://www.springerlink.com/content/x181282460853884/>

Journal Article, Academic Journal (Published)

Galeev, T. R., Romanescu, C., Li, W.-L., Wang, L.-S., Boldyrev, A. I. (2012). Observation of the Highest Coordination Number in Planar Species: Decacoordinated Ta@B₁₀⁻ and Nb@B₁₀⁻ Anions. *Angewandte Chemie International Edition*, 51(9), 2101–2105.

Journal Article, Academic Journal (Published)

Olson, J. K., Boldyrev, A. I. (2012). Electronic Transmutation: Boron Acquiring an Extra Electron Becomes "Carbon". *Chemical Physics Letters*, 523(1), 83-86.

Journal Article, Academic Journal (Published)

Galeev, T. R., Romanescu, C., Li, W.-L., Wang, L.-S., Boldyrev, A. I. (2012). Observation of the Highest Coordination Number in Planar Species: Decacoordinated Ta@B₁₀⁻ and Nb@B₁₀⁻ Anions. *Angewandte Chemie International Edition*, 51(9), 2101-2105.
<http://onlinelibrary.wiley.com/doi/10.1002/anie.201107880/abstract>

Journal Article, Academic Journal (Published)

Li, W.-L., Romanescu, C., Galeev, T. R., Piazza, Z., Boldyrev, A. I., Wang, L.-S. (2012). Transition-Metal-Centered Nine-Membered Boron Rings: M@B₉ and M@B₉. (M = Rh, Ir). *Journal of the American Chemical Society*, 8(1), 135-140.

Journal Article, Academic Journal (Published)

Ivanov, A. S., Bozhenko, K. V., Boldyrev, A. I. (2012). Peculiar Transformations in the C_xH_xP_{4-x} (x = 0-4) Series. *Journal of Chemical Theory and Computation*, 8(1), 165-168.

Journal Article, Academic Journal (Published)

Popov, I. A., Boldyrev, A. I. (2012). Deciphering Chemical Bonding in a BC₃ Honeycomb Epitaxial Sheet. *The Journal of Physical Chemistry C*, 116.
<http://pubs.acs.org/doi/full/10.1021/jp210956w>

Journal Article, Academic Journal (Published)

Olson, J. K., Boldyrev, A. I. (2011). Ab Initio Search for Global Minimum Structures of Neutral and Anionic B₄H₅ Clusters. Optical Isomerism in B₄H₅ and B₄H₅⁻. *Chemical Physics Letters*, 517, 62-67.

Journal Article, Academic Journal (Published)

Galeev, T. R., Romanescu, C., Li, W.-L., Wang, L.-S., Boldyrev, A. I. (2011). Valence isoelectronic substitution in the B₈⁻ and B₉⁻ molecular wheels by an Al dopant atom: Umbrella-like structures of AIB₇⁻ and AIB₈⁻. *Journal of Chemical Physics*, 135, 104301.

Journal Article, Academic Journal (Published)

Li, W.-L., Romanescu, C., Galeev, T. R., Wang, L.-S., Boldyrev, A. I. (2011). Aluminum Avoids the Central Position in AIB₉⁻ and AIB₁₀⁻: Photoelectron Spectroscopy and ab Initio Study. *Journal of Physical Chemistry A*, 115, 10391-10397.

Journal Article, Academic Journal (Published)

Romanescu, C., Galeev, T. R., Li, W.-L., Boldyrev, A. I., Wang, L.-S. (2011). Aromatic Metal-Centered Monocyclic Boron Rings: Co@B₈⁻ and Ru@B₉⁻. *Angewandte Chemie International Edition*, 50, 9334-9337.

Journal Article, Academic Journal (Published)

Galeev, T. R., Boldyrev, A. I. (2011). Planarity takes over in the C_xH_xP_{6-x} (x = 0–6) series at x = 4. *Physical Chemistry Chemical Physics*, 13, 20549-20556.

Journal Article, Academic Journal (Published)

Olson, J. K., Boldyrev, A. I. (2011). Ab initio characterization of the flexural B₃H₈⁻ anion found in the reversible dehydrogenation. *Computational and Theoretical Chemistry*, 967(1), 1-4.

Journal Article, Academic Journal (Published)

Sergeeva, A. P., Averkiev, B. B., Zhai, H.-J., Boldyrev, A. I., Wang, L.-S. (2011). All-boron analogues of aromatic hydrocarbons: B₁₇⁻ and B₁₈⁻. *The Journal of Chemical Physics, American Institute of Physics*, 134, 224304-1-11.

Journal Article, Academic Journal (Published)

Galeev, T. R., Chen, Q., Guo, J.-C., Bai, H., Miao, C.-Q., Lu, H.-G., Sergeeva, A. P., Li, S., Boldyrev, A. I. (2011). Deciphering the mystery of hexagon holes in an all-boron graphene α -sheet. *Physical Chemistry Chemical Physics, Royal Society of Chemistry*, 13, 11575-11578.

Journal Article, Academic Journal (Published)

Galeev, T. R., Ivanov, A. S., Romanescu, C., Li, W.-L., Bozhenko, K. V., Wang, L.-S., Boldyrev, A. I. (2011). Molecular wheel to monocyclic ring transition in boron-carbon mixed clusters C₂B₆⁻ and C₃B₅⁻. *Physical Chemistry Chemical Physics, Royal Society of Chemistry*, 13(19), 8805-8810.

Journal Article, Academic Journal (Published)

Romanescu, C., Sergeeva, A. P., Li, W.-L., Boldyrev, A. I., Wang, L.-S. (2011). Planarization of B₇⁻ and B₁₂⁻ Clusters by Isoelectronic Substitution: AIB₆⁻ and AIB₁₁⁻. *Journal of the American Chemical Society, American Chemical Society*, 133(22), 8646–8653.
<http://pubs.acs.org/doi/full/10.1021/ja2012438>

Journal Article, Academic Journal (Published)

Galeev, T. R., Boldyrev, A. I. (2011). Recent advances in aromaticity and antiaromaticity in transition-metal systems. *Annual Report Section C, Physical Chemistry, Royal Society of Chemistry*, 107, 124-147.

Journal Article, Academic Journal (Published)

Martínez-Guajardo, G., Sergeeva, A. P., Boldyrev, A. I., Heine, T., Ugalde, J. M., Merino, G. (2011). Unravelling phenomenon of internal rotation in B13+ through chemical bonding analysis. *Chemical Communications*, 47, 6242-6244.

Journal Article, Academic Journal (Published)

Olson, J. K., Boldyrev, A. I. (2011). Ab Initio Search for Global Minimum Structures of Neutral and Anionic B4H4 Clusters. *Chemical Physics*, 379, 1-5.

Journal Article, Academic Journal (Published)

Pokhodnya, K., Olsen, C., Dai, X., Schilz, D. L., Boudjouk, P., Sergeeva, A. P., Boldyrev, A. I. (2011). Flattening a puckered cyclohexasilane ring by suppression of the pseudo-Jahn-Teller effect. *Journal of Chemical Physics*, 134.

Journal Article, Academic Journal (Published)

Alexandrova, A. N., Boldyrev, A. I., Li, X., Sarkas, H. W., Hendricks, J. H., Arnold, S. T., Bowen, K. H. (2011). Lithium cluster anions: Photoelectron spectroscopy and ab initio calculations. *The Journal of Chemical Physics, American Institute of Physics*, 134(4), 044322-1-8. http://jcp.aip.org/resource/1/jcpsa6/v134/i4/p044322_s1

Journal Article, Academic Journal

Romanescu, C., Galeev, T., Li, W.-L., Boldyrev, A. I., Wang, L.-S. (2013). Transition-Metal-Centered Monocyclic Boron Wheel Clusters (M@Bn): A New Class of Aromatic Borometallic Compounds. *Acc. Chem. Res.*

Chang, Cheng Wei T.

Journal Article, Professional Journal (Published)

Zhang, Q., Chang, C. W. T. (2015). Divergent and Facile Lewis Acid-Mediated Synthesis of N-Alkyl 2-aminomethylene-1,3-indanediones and 2-Alkylamino-1,4-Naphthoquinones. *Tetrahedron Lett*, 56, 893.

Journal Article, Professional Journal (Published)

Shrestha, J., Subedi, Y., Chen, L., Chang, C. W. T. (2015). Mode of Action Study of Cationic Anthraquinone Analog: A New Class of Highly Potent Anti-cancer Agent. *MedChemComm*, 2012.

Journal Article, Professional Journal (Published)

Fosso, M., AlFindee, M., Zhang, Q., Nziko, V., Kawasaki, Y., Shrestha, S., Bearss, J., Gregory, R., Takemoto, J., Chang, C. W. T. (2015). Structure–Activity Relationships for Antibacterial to Antifungal Conversion of Kanamycin to Amphiphilic Analogues. *J Org Chem*, 80, 4398.

Journal Article, Academic Journal (Published)

Shrestha, S. K., Grilley, M. M., Anderson, T., Dhiman, C., Oblad, J., Chang, C. W. T., Sorensen, K. N., Takemoto, J. Y. (2015). In vitro antifungal synergy between amphiphilic aminoglycoside K20 and azoles against *Candida* species and *Cryptococcus neoformans*. *Med Mycol*. <http://www.ncbi.nlm.nih.gov/pubmed/26260746>

Journal Article, Professional Journal (Published)

Zhang, Q., Peng, X., Grilley, M. M., Takemoto, J. Y., Chang, C. W. T. (2015). Using Fluorogenic Probes for the Investigation of Selective Biomass Degradation by Fungi. *Green Chem*, 17, 1918-1925.

Journal Article, Academic Journal (Published)

Shrestha, S. K., Chang, C. W. T., Meissner, N., Oblad, J., Shrestha, J. P., Sorensen, K. N., Grilley, M. M., Takemoto, J. Y. (2014). Antifungal amphiphilic aminoglycoside K20: bioactivities and mechanism of action. *Frontiers in Microbiology*, 5(271), 1-12. http://www.frontiersin.org/Journal/Abstract.aspx?s=727&name=fungi_and_their_interactions&ART_DOI=10.3389/fmicb.2014.00671

Journal Article, Professional Journal (Published)

Nziko, Fosso, M., Chang, C. W. T. (2014). Quantitative structure activity relationship analysis of antibacterial cationic anthraquinone analogs using Hansch and Fujita models. *Med. Chem. Res*, 23, 5058-5062.

Journal Article, Professional Journal (Published)

Shrestha, J., Fosso, M. Y., Bearss, J., Chang, C. W. T. (2014). Synthesis and anticancer structure activity relationship investigation of cationic anthraquinone analogs. *Eur. J. Med. Chem.*, 77, 96-102.

Journal Article, Professional Journal (Published)

Zhang, Q., Shrestha, J., Chang, C. W. T. (2014). Synthesis of bioactive 1-alkyl-1H-naphtho[2,3-d][1,2,3]triazole-4,9-diones and N-aryl-2-aminomethylene-1,3-indanediones using water as the solvent. *Tetrahedron Lett*, 55, 1839-1842.

Journal Article, Professional Journal (Published)

Udumula, U., Ham, Y. W., Fosso, M., Chen, K. Y., Rai, R., Zhang, J., Li, J., Chang, C. W. T. (2013). Investigation of Antibacterial Mode of Action for Traditional and Amphiphilic Aminoglycosides. *Bioorg Med Chem Lett*, 23, 1671-1675.

Journal Article, Professional Journal (Published)

Ito, T., Chen, D., Chang, C. W. T., Kenmochi, T., Saito, T., Suzuki, S., Takemoto, J. Y. (2013). Meso-biliverdin IXa and Biliverdin IX Provide Cytoprotection of Rat Pancreatic Islets. *Frontiers in Pharmacology*(4), 1-8.

Journal Article, Professional Journal (Published)

Shrestha, J., Chang, C. W. T. (2013). Safe and Easy Route for the Synthesis of 1,3-Dimethyl-1,2,3-triazolium Salt and Investigation of Its Anticancer Activities. *Bioorg Med Chem Lett*, 23, 5909-5911.

Journal Article, Academic Journal (Published)

Lee, S. T., Green, B. T., Welch, K. D., Jordan, G. T., Zhang, Q., Panter, K. E., Hughe, D., Chang, C. W. T., Pfister, J. A., Gardner, D. R. (2013). Stereoselective Potencies and Relative Toxicities of γ -Coniceine, and N-Methylconiine Enantiomers. *Chemical Research in Toxicology*, 26, 616-621.

Journal Article, Academic Journal (Published)

Shrestha, S., Grilley, M. M., Fosso, M. Y., Chang, C. W. T., Takemoto, J. Y. (2013). Membrane lipid-modulated mechanism of action and non-cytotoxicity of novel fungicide aminoglycolipid FG08. *PLoS One*.

Journal Article, Academic Journal (Published)

Shrestha, S., Grilley, M. M., Fosso, M. Y., Chang, C. W. T., Takemoto, J. Y. (2013). Membrane Lipid-Modulated Mechanism of Action and Non-Cytotoxicity of Novel Fungicide Aminoglycoside FG08. *PLoS one*, 8(9), e73843.

Journal Article, Professional Journal (Published)

Fosso, M., Nziko, V. P. N., Chang, C. W. T. (2012). Chemical Synthesis of N-Aryl Glycosides. *J. Carbohydr. Chem.*, 31, 603.

Journal Article, Academic Journal (Published)

Lee, S. T., Panter, K. E., Gardner, D. R., Green, B. T., Welch, K. D., Zhang, J., Chang, C. W. T. (2012). Development of a monoclonal antibody-based ELISA for the hedgehog inhibitors cyclopamine and cyclopamine-KAAD. *J. Pharmaceut. Biomed. Anal.*, 66, 282-286.

Journal Article, Professional Journal (Published)

Fosso, M., Chen, K. Y., Gregory, R., Chang, C. W. T. (2012). Library Synthesis and Antibacterial Investigation of Cationic Anthraquinone Analogs. *ACS*, 14, 231.

Journal Article, Professional Journal (Published)

Chan, K. Y., Zhang, J., Chang, C. W. T. (2011). Mode of Action Investigation for the Antibacterial Cationic Anthraquinone Analogs. *Bioorg. Med. Chem. Lett.*, 21, 6353.

Journal Article, Academic Journal (Submitted)

Lee, S. T., Welch, K., Panter, K. E., Gardner, D., Garrossian, M., Chang, C. W. T. (2014). Cyclopamine: From Cyclops Lambs to Cancer Treatment. *J. Agric. Food Chem.*

Journal Article, Academic Journal (Submitted)

Zhang, S., Wang, S., Zhang, Q., Chang, C. W. T., Zhan, J. Three new derivatives of cephalosporin P1 and their antibacterial activity. *Pharmacognosy Magazine*, 5806-5809.

Journal Article, Professional Journal (Submitted)

Osner, Z. R., Nyamjav, D., Liang, Y., Chang, C. W. T., Gomez, J., Long, P., Kelly, J., Becker, D., Holz, R. C. (2013). Nano-Patterned Carbohydrate Interfaces for Bacterial Cell Capture. *Langmuir*.

Journal Article, Academic Journal (Published)

Zhang, J., Redman, N., Litke, P., Zeng, J., Zhan, J., Chan, K. Y., Chang, C. W. T. (2011). Synthesis and Antibacterial Activity Study of a Novel Class of Cationic Anthraquinone Analogs. *Bioorganic Medicinal Chemistry*, 19, 498-503.

Journal Article, Academic Journal (Published)

Burgess, J. L., Jones, H. B., Kumar, P., Toth, R., Middaugh, C. Russell, Antony, E., Dickenson, N. (2016). Spa47 is an oligomerization-activated type three secretion system (T3SS) ATPase from *Shigella flexneri*. *Protein Science*, 25, 1037-1048.

Ensign, Scott A.

Journal Article, Academic Journal (Published)

Pandey, A. S., Mulder, D. W., Ensign, S. A., Peters, J. W. (2011). Structural basis for carbon dioxide binding by 2-ketopropyl coenzyme M oxidoreductase/carboxylase. *FEBS Letters*, 585, 459-464.

Journal Article, Academic Journal (Published)

Kofoed, M. A., Wampler, D. A., Pandey, A. S., Peters, J. W., Ensign, S. A. (2011). Roles of the redox active disulfide, and histidine residues forming a catalytic dyad, in reactions catalyzed by 2-Ketopropyl-Coenzyme M Oxidoreductase/Carboxylase. *The Journal of Bacteriology*, 193, 4904-4913.

Farrelly, David

Journal Article, Academic Journal (Published)

Wairegi, A., Farrelly, D. (2015). Genetic Algorithm Diffusion Monte Carlo with Importance Sampling. *Chemical Physics Letters*, 619, 71.

Journal Article, Academic Journal (Published)

Wairegi, A., Suarez, A. G., Lee, E. A., Burbanks, A., Farrelly, D. (2014). Microscopic Superfluidity in helium-4 clusters stirred by a rotating impurity molecule. *Physical Review Letters*, 112, 143401.

Journal Article, Academic Journal (Published)

Ramilowski, J. A., Farrelly, D. (2012). Fixed node diffusion Monte Carlo using a genetic algorithm: A study of the CO-He_N complex, N = 1 - 10. *Physical Chemistry Chemical Physics*, 14(22), 8123-8136.

Journal Article, Academic Journal (Published)

Gamboa, A., Ramilowski, J. A., Benito, R., Farrelly, D. (2011). Renormalization of the rotational constants of an ammonia molecule seeded into a helium-4 droplet. *Chemical Physics Letters*, 502, 14-22.

Hengge, Alvan C.

Journal Article, Academic Journal (Published)

Moise, G., Gallup, N. M., Alexandrova, A. N., Hengge, A. C., Johnson, S. J. (2015). Conservative Tryptophan Mutants of the Protein Tyrosine Phosphatase YopH Exhibit Impaired WPD-Loop Function and Crystallize with Divanadate Esters in Their Active Sites. *Biochemistry*, 54(42), 6490-6500.

Journal Article, Academic Journal (Published)

Kuznetsov, V. I., Hengge, A. C. (2013). New Functional Aspects of the Atypical Protein Tyrosine Phosphatase VHZ. *Biochemistry*, 52(45), 8012-8025.

Journal Article, Academic Journal (Published)

Hengge, A. C., Kuznetsov, V. I., Alexandrova, A. N. (2012). Metavanadate at the Active Site of the Phosphatase VHZ. *Journal of the American Chemical Society*, 134(35), 14298-14301.

Journal Article, Academic Journal (Published)

Kuznetsov, V. I., Hengge, A. C., Johnson, S. J. (2012). New aspects of the phosphatase VHZ revealed by a high-resolution structure with vanadate and substrate screening. *Biochemistry*, 51(49), 9869-9879.

Hevel, Joan M.

Journal Article, Academic Journal (Published)

Gui, S., Gathiaka, S., Li, J., Qu, J., Acevedo, O., Hevel, J. M. (2014). A remodeled protein arginine methyltransferase 1 (PRMT1) generates symmetric dimethylarginine. *Journal of Biological Chemistry*, 289, 9320-7.

Journal Article, Academic Journal (Published)

Wang, C., Zhu, Y., Caceres, T., Liu, L., Peng, J., Wang, J., Chen, X., Zhang, Z., Zuo, X., Gong, Q., Teng, M., Hevel, J. M., Wu, J., Shi, Y. (2014). Structural Determinants for the

Strict Monomethylation Activity by Trypanosoma brucei Protein Arginine Methyltransferase 7. *Structure*.

Journal Article, Academic Journal (Published)

Gui, S., Wooderchak, W. L., Zhang, T., Chen, D., Daly, M., Zhou, Z. S., Hevel, J. M. (2012). Substrate-induced control of product formation by protein arginine methyltransferase 1. *Biochemistry*, 52, 199-209.

Journal Article, Academic Journal (Published)

Gui, L., Wooderchak, W. L., Daly, M. P., Porter, P. J., Johnson, S. J., Hevel, J. M. (2011). Investigation of the Molecular Origins of Protein Arginine Methyltransferase I (PRMT1) Product Specificity Reveals a Role for Two Conserved Methionine Residues. *Journal of Biological Chemistry*, 286(33), 29118-26.

Journal Article, Academic Journal (Published)

Morales, Y., Cáceres, T., May, K., Hevel, J. M. (2016). Biochemistry and regulation of the protein arginine methyltransferases (PRMTs). *Archives of biochemistry and biophysics*, 590, 138-52.

Journal Article, Academic Journal (Published)

Morales, Y., Nitzel, D. V., Price, O. M., Gui, S., Li, J., Qu, J., Hevel, J. M. (2015). Redox Control of Protein Arginine Methyltransferase 1 (PRMT1) Activity. *The Journal of biological chemistry*, 290(24), 14915-26.

Johnson, Sean J.

Journal Article, Academic Journal (Published)

Losh, J. S., King, A. K., Bakelar, J., Taylor, L., Loomis, J., Rosenzweig, J. A., Johnson, S. J., van Hoof, A. (2015). Interaction between the RNA-dependent ATPase and poly(A) polymerase subunits of the TRAMP complex is mediated by short peptides and important for snoRNA processing. *Nucleic Acids Research*, 43(3), 1848-1858.

Journal Article, Academic Journal (Published)

Taylor, L., Jackson, R. N., Rexhepaj, M., King, A. K., Lott, L. K., van Hoof, A., Johnson, S. J. (2014). The Mtr4 ratchet helix and arch domain both function to promote RNA unwinding. *Nucleic Acids Research*, 42(22), 13861-13872.

Journal Article, Academic Journal (Published)

Bakelar, J. W., Sliwa, D. A., Johnson, S. J. (2013). Crystal structures of S-HPCDH reveal determinants of stereospecificity for R- and S-hydroxypropyl-coenzyme M dehydrogenases. *Archives of Biochemistry and Biophysics*.

Journal Article, Academic Journal (Published)

Zeng, J., Lytle, A. K., Gage, D., Johnson, S. J., Zhan, J. (2013). Specific chlorination of isoquinolines by a fungal flavin-dependent halogenase. *Bioorganic and Medicinal Chemistry Letters*, 23(4), 1001-1003.

Journal Article, Academic Journal (Published)

Johnson, S. J., Jackson, R. N. (2013). Structures of Ski2-like RNA helicases: common themes and complex assemblies. *RNA Biology*, 10(1), 33-43.

Scheiner, Stephen I.

Journal Article, Professional Journal (Published)

Nepal, B., Scheiner, S. I. (2016). Building a Better Halide Receptor. Optimum Choice of Spacer, Binding Unit, and Halosubstitution. *ChemPhysChem*, 17, 836-844.

Journal Article, Professional Journal (Published)

Nziko, v., Scheiner, S. I. (2016). Catalysis of the Aza-Diels-Alder Reaction by Hydrogen and Halogen Bonds. *J. Org. Chem.*, 81, 2589-2597.

Journal Article, Professional Journal (Published)

Nziko, V., Scheiner, S. I. (2016). Comparison of π -Hole Tetrel Bonding with σ -Hole Halogen Bonds in Complexes of XCN (X = F, Cl, Br, I) and NH₃. *Phys. Chem. Chem. Phys.*, 18, 3581-3590.

Journal Article, Professional Journal (Published)

Nepal, b., Scheiner, S. I. (2016). Enhancing the Reduction Potential of Quinones via Complex Formation. *J. Org. Chem.*, 81, 4316-4324.

Journal Article, Academic Journal (Published)

Kasende, O. E., Muya, J. T., Paul N. Nziko, Vincent, Scheiner, S. I. (2016). Hydrogen bonded and stacked geometries of the temozolomide dimer. *Journal of Molecular Modeling*, 22(4), 1–9. <http://dx.doi.org/10.1007/s00894-016-2934-z>

Journal Article, Professional Journal (Published)

Kasende, O., Matondo, A., Muya, J. T., Scheiner, S. I. (2016). Interaction Between Temozolomide and HCl: Preferred Binding Sites. *Comp. Theor. Chem.*, 1075, 82-86.

Journal Article, Professional Journal (Published)

Fick, r., kroner, g., nepal, b., magnani, r., Horowitz, s., Houtz, R., Scheiner, S. I., Trievel, R. (2016). Sulfur - Oxygen Chalcogen Bonding Mediates AdoMet Recognition in the Lysine Methyltransferase SET7/9. *ACS Chem. Biol.*, 11, 748-754.

Journal Article, Professional Journal (Published)

Nepal, B., Scheiner, S. I. (2015). Angular Dependence of Hydrogen Bond Energy in Neutral and Charged Systems containing CH and NH Proton Donors. *Chem. Phys. Lett.*, 630, 6-11.

Journal Article, Professional Journal (Published)

Nepal, B., Scheiner, S. I. (2015). Anionic CH \cdots X- Hydrogen Bonds. Origin of their Strength, Geometry, and Other Properties. *Chem. Eur. J.*, 21, 1474-1481.

Journal Article, Academic Journal (Published)

Nepal, B., Scheiner, S. I. (2015). Competitive Halide Binding by Halogen Versus Hydrogen Bonding: Bis-triazole Pyridinium. *Chemistry – A European Journal*, 21(38), 13330–13335. <http://dx.doi.org/10.1002/chem.201501921>

Journal Article, Professional Journal (Published)

Scheiner, S. I. (2015). Dissection of the Factors Affecting Formation of a CH \cdots O H-bond. A Case Study. *Crystals*, 5, 327-345.

Journal Article, Professional Journal (Published)

Nziko, v. d. P. N., Scheiner, S. I. (2015). Interactions between Thiourea and Imines. Prelude to Catalysis. *J. Org. Chem.*, 54, 10334–10341.

Journal Article, Professional Journal (Published)

Nziko, v. d. P. N., Scheiner, S. I. (2015). Intramolecular S··O Chalcogen Bond as Stabilizing Factor in Geometry of Substituted Phenyl-SF₃ Molecules. *J. Org. Chem.*, *80*, 2356-2363.

Journal Article, Professional Journal (Published)

Nepal, B., Scheiner, S. I. (2015). Long-Range Behavior of Noncovalent Bonds. Neutral and Charged H-Bonds, Pnicogen, Chalcogen, and Halogen Bonds. *Chem. Phys.*, *456*, 34-40.

Journal Article, Professional Journal (Published)

Nepal, b., Scheiner, S. I. (2015). Microsolvation of Anions by Molecules Forming CH··X-Hydrogen Bonds. *Chem. Phys.*, *463*, 137-144.

Journal Article, Professional Journal (Published)

Kasende, O., Muya, J. T., Scheiner, S. I. (2015). Regioselectivity of the Interaction of Temozolomide with Borane and Boron Trifluoride. *Struct. Chem.*, *26*, 1359-1365.

Journal Article, Professional Journal (Published)

nepal, b., Scheiner, S. I. (2015). Substituent Effects on the Binding of Halides by Neutral and Dicationic Bis-Triazolium Receptors. *J. Phys. Chem. A*, *119*, 13064–13073.

Journal Article, Professional Journal (Published)

nziko, v., Scheiner, S. I. (2015). S··π Chalcogen Bonds between SF₂ or SF₄ and C-C Multiple Bonds. *J. Phys. Chem. A*, *119*, 5889-5897.

Journal Article, Professional Journal (Published)

nziko, v., Scheiner, S. I. (2014). Chalcogen Bonding between Tetravalent SF₄ and Amines. *J. Phys. Chem. A*, *118*, 10849–10856.

Journal Article, Professional Journal (Published)

Lone, B., Scheiner, S. I., Kar, T. (2014). Competition between Carboxylic and Phenolic Groups for the Preferred Sites at the Periphery of Graphene – A DFT study. *Carbon*, *80*, 405-418.

Journal Article, Professional Journal (Published)

Adhikari, u., Scheiner, S. I. (2014). Competition between Lone Pair-π, Halogen Bond, and Hydrogen Bond in Adducts of Water with Perhalogenated Alkenes C₂ClnF_{4-n} (n = 0-4). *Chem. Phys.*, *440*, 53-63.

Journal Article, Professional Journal (Published)

Adhikari, U., Scheiner, S. I., Roy, A. K., Kar, T. (2014). Do phenolic and carboxylic groups coexist at the tips of oxidized single-wall carbon nanotubes (o-SWNTs)? *Carbon*, *73*, 194-205.

Journal Article, Professional Journal (Published)

Nepal, B., Scheiner, S. I. (2014). Effect of Ionic Charge upon the CH··π Hydrogen Bond. *J. Phys. Chem. A*, *118*, 9575-9587.

Journal Article, Professional Journal (Published)

Scheiner, S. I., Adhikari, U. (2014). Effects of Charge and Substituent on the S···N Chalcogen Bond. *J. Phys. Chem. A*, *118*, 3183-3192.

Journal Article, Professional Journal (Published)

Horowitz, S., Adhikari, U., Dirk, L., Del Rizzo, P. A., Mehl, R. A., Houtz, R. L., Al-Hashimi, H. M., Scheiner, S. I., Trievel, R. C. (2014). Manipulating Unconventional CH-based Hydrogen Bonding in a Methyltransferase via Unnatural Amino Acid Mutagenesis. *ACS Chemical Biology*, *9*, 1692-1697.

Journal Article, Professional Journal (Published)

Horowitz, S., Dirk, L.M.A., Yesselman, J.D., Nitz, J.S., Adhikari, U., Mehl, R.A., Scheiner, S. I., Houtz, R.L., Al-Hashimi, H.M., Trievel, R.C. (2013). Conservation and Functional Importance of Carbon-Oxygen Hydrogen Bonding in AdoMet-dependent Methyltransferases. *J. Am. Chem. Soc.*, 135, 15536-15548.

Journal Article, Professional Journal (Published)

Scheiner, S. I., Adhikari, U. (2013). First Steps in Growth of a Polypeptide Toward β -Sheet Structure. *J. Phys. Chem. B*, 117, 11575-11583.

Journal Article, Professional Journal (Published)

Adhikari, U., Scheiner, S. I. (2013). Preferred Configurations of Peptide-Peptide Interactions. *J. Phys. Chem. A*, 117, 489-496.

Journal Article, Professional Journal (Published)

Kar, T., Scheiner, S. I., Adhikari, U., Roy, A. (2013). Site Preferences of Carboxyl Groups on the Periphery of Graphene and their Characteristic IR Spectra. *J Phys. Chem. C*, 117, 18206-18215.

Journal Article, Academic Journal (Published)

Adhikari, U., Scheiner, S. I. (2013). The Magnitude and Mechanism of Charge Enhancement of CH \cdots O H-bonds. *J. Phys. Chem. A*, 117, 10551-10562.

Journal Article, Professional Journal (Published)

Scheiner, S. I., adhikari, u. (2012). Contributions of Various Noncovalent Bonds to the Interaction between an Amide and S-Containing Molecules. *ChemPhysChem*, 13, 3535-3541.

Journal Article, Professional Journal (Published)

Scheiner, S. I., Adhikari, U. (2012). Effects of Carbon Chain Substituent on the P \cdots N Noncovalent Bond. *Chem. Phys. Lett.*, 536, 30-33.

Journal Article, Professional Journal (Published)

Scheiner, S. I., upendra, a. (2012). Sensitivity of Pnictogen, Chalcogen, Halogen and H-Bonds to Angular Distortions. *Chem. Phys. Lett.*, 532, 31-35.

Journal Article, Professional Journal (Published)

Scheiner, S. I., upendra, a. (2012). Substituent Effects on Cl \cdots N, S \cdots N, and P \cdots N Noncovalent Bonds. *J. Phys. Chem. A*, 116, 3487-3497.

Journal Article, Professional Journal (Published)

Chen, S., Scheiner, S. I., Kar, T., Adhikari, U. (2012). Theoretical study on relationship between structure of mercapto-triazole derivatives and inhibition performance. *Int. J. Electrochem. Sci.*, 7, 7128-7139.

Journal Article, Professional Journal (Published)

Scheiner, S. I., Adhikari, U. (2011). Abilities of Different Electron Donors (D) to Engage in a P \cdots D Noncovalent Interaction. *J. Phys. Chem. A*, 115, 11101 - 11110.

Journal Article, Professional Journal (Published)

Scheiner, S. I., Adhikari, U. (2011). Comparison of P \cdots D (D=P,N) with Other Noncovalent Bonds in Molecular Aggregates. *J. Chem. Phys.*, 135, 184306.

Journal Article, Professional Journal (Published)

Scheiner, S. I., Adhikari, U. (2011). The S \cdots N Noncovalent Interaction: Comparison with Hydrogen and Halogen Bonds. *Chem. Phys. Lett.*, 514, 36-39.

Journal Article, Professional Journal (Published)

Scheiner, S. I., Adhikari, U. (2011). The S···N Noncovalent Interaction: Comparison with Hydrogen and Halogen Bonds. *Chem. Phys. Lett.*, 514, 36-39.

Seefeldt, Lance C.

Journal Article, Academic Journal (Published)

Lukoyanov, D., Yang, Z.-Y., Khadka, N., Dean, D. R., Seefeldt, L., Hoffman, B. M. (2015). Identification of a Key Catalytic Intermediate Demonstrates That Nitrogenase Is Activated by the Reversible Exchange of N₂ for H₂. *Journal of the American Chemical Society*. <http://pubs.acs.org/doi/abs/10.1021/jacs.5b00103>

Journal Article, Academic Journal (Published)

Wills, M., McCurdy, A., Ogborn, M., Wahlen, B., Quinn, J., Pease, L., Seefeldt, L. (2014). Improving Energetics of Triacylglyceride Extraction from Wet Oleaginous Microbes. *Bioresource Technology*, 167, 416-424.

Journal Article, Academic Journal (Published)

McCurdy, A., Higham, A., Morgan, M., Quinn, J., Seefeldt, L. (2014). Two-step Process for Production of Biodiesel Blends from Oleaginous Yeast and Microalgae. *Fuel*, 137, 269-276.

Journal Article, Academic Journal (Published)

Shaw, S., Lukoyanov, D., Danyal, K., Dean, D. R., Hoffman, B. M., Seefeldt, L. (2014). Nitrite and Hydroxylamine as Nitrogenase Substrates: Mechanistic Implications for the Pathway of N₂ Reduction. *Journal of the American Chemical Society*, 136(36), 12776–12783. <http://dx.doi.org/10.1021/ja507123d>

Journal Article, Academic Journal (Published)

Hoffman, B. M., Lukoyanov, D., Yang, Z.-Y., Dean, D. R., Seefeldt, L. (2014). Mechanism of nitrogen fixation by nitrogenase: the next stage. *Chemical Reviews*, 114(8), 4041–4062. <http://dx.doi.org/10.1021/cr400641x>

Journal Article, Academic Journal (Published)

Smith, D., Danyal, K., Raugei, S., Seefeldt, L. (2014). Substrate channel in nitrogenase revealed by a molecular dynamics approach. *Biochemistry*, 53(14), 2278–2285. <http://dx.doi.org/10.1021/bi401313j>

Journal Article, Academic Journal (Published)

Lukoyanov, D., Yang, Z.-Y., Duval, S., Danyal, K., Dean, D. R., Seefeldt, L., Hoffman, B. M. (2014). A confirmation of the quench-cryoannealing relaxation protocol for identifying reduction states of freeze-trapped nitrogenase intermediates. *Inorganic Chemistry*, 53, 3688–3693. <http://dx.doi.org/10.1021/ic500013c>

Journal Article, Professional Journal (Published)

Wahlen, B. D., Morgan, M. R., McCurdy, A. T., Willis, R. M., Dye, D. J., Bugbee, B. G., Wood, B. D., Seefeldt, L. (2013). Biodiesel from microalgae, yeast, and bacteria: engine performance and exhaust emissions. *Energy Fuels*, 27, 220-228.

Journal Article, Professional Journal (Published)

Duval, S., Danyal, K., Shaw, S., Lytle, A. K., Dean, D. R., Hoffman, B. M., Antony, E., Seefeldt, L. (2013). Electron transfer precedes ATP hydrolysis during nitrogenase catalysis. *Proc. Natl. Acad. Sci. USA*, 110, 16414-16419.

Journal Article, Professional Journal (Published)

Seefeldt, L., Yang, Z. Y., Duval, S., Dean, D. R. (2013). Nitrogenase reduction of carbon-containing compounds. *Biochim. Biophys. Acta*, 1827, 1102-1111.

Journal Article, Professional Journal (Published)

Yang, Z. Y., Khadka, N., Lukoyanov, D., Hoffman, B. M., Dean, D. R., Seefeldt, L. (2013). On reversible H₂ loss upon N₂ binding to FeMo-cofactor of nitrogenase. *Proc. Natl. Acad. Sci. USA*, 110, 16327-16332.

Journal Article, Professional Journal (Published)

Moure, V. R., Danyal, K., Wendroth, S., Muller-Santos, M., Pedrosa, F. O., Scarduelli, M., Souza, E. M., Seefeldt, L. (2013). The nitrogenase regulatory enzyme dinitrogenase reductase ADP-ribosyltransferase (DraT) is activated by direct interaction with the signal transduction protein GlnB. *J. Bacteriol.*, 195, 279-286.

Journal Article, Professional Journal (Published)

Adams, C., Godfrey, V., Wahlen, B., Seefeldt, L., Bugbee, B. G. (2013). Understanding precision nitrogen stress to optimize the growth and lipid content tradeoff in oleaginous green microalgae. *Bioresource Technol.*, 131, 188-194.

Journal Article, Professional Journal (Published)

Yang, Z. Y., Moure, V. R., Dean, D. R., Seefeldt, L. (2012). Carbon dioxide reduction to methane and coupling with acetylene to form propylene catalyzed by remodeled nitrogenase. *Proc. Natl. Acad. Sci. USA*, 109, 19644-19648.

Journal Article, Professional Journal (Published)

Barney, B. M., Wahlen, B. D., Garner, E., Wei, J., Seefeldt, L. (2012). Differences in substrate specificities of five bacterial was ester synthases. *Appl. Environ. Microbiol.*, 78, 5734-5745.

Journal Article, Professional Journal (Published)

Mayweather, D., Danyal, K., Dean, D. R., Seefeldt, L., Hoffman, B. M. (2012). Temperature invariance of the nitrogenase electron transfer mechanism. *Biochemistry*, 51, 8391-8398.

Journal Article, Professional Journal (Published)

Lukoyanov, D., Yang, Z. Y., Barney, B. M., Dean, D. R., Seefeldt, L., Hoffman, B. M. (2012). Unification of reaction pathway and kinetic scheme for N₂ reduction catalyzed by nitrogenase. *Proc. Natl. Acad. Sci. USA*, 109, 5583-5587.

Journal Article, Professional Journal (Published)

Doan, P. E., Telser, J., Barney, B. M., Igarashi, R. Y., Dean, D. R., Seefeldt, L., Hoffman, B. M. (2011). (57)Fe ENDOR spectroscopy and 'electron inventory' analysis of the nitrogenase E(4) intermediate suggest the metal-ion core of FeMo-cofactor cycles through only one redox couple. *J. Am. Chem. Soc.*, 133, 17329-17340.

Journal Article, Professional Journal (Published)

Danyal, K., Dean, D. R., Hoffman, B. M., Seefeldt, L. (2011).) Electron transfer within nitrogenase: evidence for a deficit spending mechanism. *Biochemistry*, 50, 9255-9263.

Journal Article, Professional Journal (Published)

Willis, R. M., Wahlen, B. D., Seefeldt, L., Barney, B. M. (2011). Characterization of a fatty acyl-CoA reductase from *Marinobacter aquaeolei* VT8: A bacterial enzyme catalyzing the reduction of fatty acyl-CoA to fatty alcohol. *Biochemistry*, 50, 10550-10558.

Journal Article, Professional Journal (Published)

Lukoyanov, D., Dkianov, S. A., Yang, Z. H., Barney, B. M., Samoilova, R. I., Narasimhulu, K., Dean, D. R., Seefeldt, L., Hoffman, B. M. (2011). ENDOR/HYSCORE studies of the common intermediate trapped during nitrogenase reduction of N₂H₂, CH₃N₂H, and N₂H₄ support an alternating reaction pathway for N₂ reduction. *J. Am. Chem. Soc.*, *133*, 11655-11664.

Journal Article, Professional Journal (Published)

Yang, Z., Dean, D. R., Seefeldt, L. (2011). Molybdenum nitrogenase catalyzes the reduction and coupling of CO to form hydrocarbons. *J. Biol. Chem.*, *286*, 19417-19421.

Journal Article, Academic Journal (Published)

Yang, Z. Y., Seefeldt, L., Dean, D. R., Cramer, S. P., George, S. J. (2011). Steric control of the Hi-CO MoFe nitrogenase complex revealed by stopped-flow infra-red spectroscopy. *Angewandte Chemie International Edition*, *50*, 272-275.

Journal Article, Academic Journal (Accepted)

Wahlen, B. D., Willis, R. M., Seefeldt, L. (2011). Biodiesel production by simultaneous extraction and conversion of total lipids from microalgae, cyanobacteria, and wild-mixed cultures. *Bioresource Technology*, *102*, 2724-2730.

Journal Article, Academic Journal (Published)

Jena, U., McCurdy, A. T., Warren, A., Summers, H., Ledbetter, R. N., Hoekman, S. K., Seefeldt, L., Quinn, J. (2015). Oleaginous yeast platform for producing biofuels via co-solvent hydrothermal liquefaction. *Biotechnology for Biofuels*, *8*(1).
<http://www.biotechnologyforbiofuels.com/content/8/1/167>

Journal Article, Academic Journal (Published)

Summers, H. M., Ledbetter, R. N., McCurdy, A. T., Morgan, M. R., Seefeldt, L., Jena, U., Kent Hoekman, S., Quinn, J. (2015). Techno-economic feasibility and life cycle assessment of dairy effluent to renewable diesel via hydrothermal liquefaction. *Bioresource Technology*, *196*, 431-440.
<http://www.sciencedirect.com/science/article/pii/S0960852415010391>

Journal Article, Academic Journal (Published)

Danyal, K., Rasmussen, A. J., Keable, S. M., Inglet, B. S., Shaw, S., Zadvornyy, O. A., Duval, S., Dean, D. R., Raugei, S., Peters, J. W., Seefeldt, L. (2015). Fe Protein-Independent Substrate Reduction by Nitrogenase MoFe Protein Variants. *Biochemistry*, *54*(15), 2456-2462. <http://dx.doi.org/10.1021/acs.biochem.5b00140>

Journal Article, Academic Journal (Published)

Adams, C., Godfrey, V., Wahlen, B., Seefeldt, L., Bugbee, B. G. (2013). Understanding precision nitrogen stress to optimize the growth and lipid content tradeoff in oleaginous green microalgae. *Bioresource technology*, *131*, 188-194.

Journal Article, Academic Journal (Published)

Wahlen, B. D., Morgan, M. R., McCurdy, A. T., Willis, R. M., Morgan, M. D., Dye, D. J., Bugbee, B. G., Wood, B. D., Seefeldt, L. (2012). Biodiesel from microalgae, yeast, and bacteria: engine performance and exhaust emissions. *Energy & Fuels*, *27*(1), 220-228.

Sun, Yujie

Journal Article, Academic Journal (Published)

Jiang, N., You, B., Sheng, M., Sun, Y. (2016). Bifunctionality and Mechanism of Electrodeposited Nickel-Phosphorous Films for Efficient Overall Water Splitting. *ChemCatChem*, *8*(1), 106-112.

Journal Article, Academic Journal (Published)

You, B., Sun, Y. (2016). Hierarchically Porous Nickel Sulfide Multifunctional Superstructures. *Advanced Energy Materials*, n/a-n/a.

Journal Article, Academic Journal (Published)

You, B., Jiang, N., Sun, Y. (2016). Morphology-activity correlation in hydrogen evolution catalyzed by cobalt sulfides. *Inorganic Chemistry Frontiers*.

Journal Article, Academic Journal (Published)

Jiang, N., Tang, Q., Sheng, M., You, B., Jiang, D.-e., Sun, Y. (2016). Nickel sulfides for electrocatalytic hydrogen evolution under alkaline conditions: a case study of crystalline NiS, NiS₂, and Ni₃S₂ nanoparticles. *Catalysis Science & Technology*, 6(4), 1077-1084.

Journal Article, Academic Journal (Published)

Sheng, M., Jiang, N., Gustafson, S., You, B., Ess, D. H., Sun, Y. (2015). A nickel complex with a biscarbene pincer-type ligand shows high electrocatalytic reduction of CO₂ over H₂O. *Dalton Transactions*, 44(37), 16247-16250.

Journal Article, Academic Journal (Published)

You, B., Jiang, N., Sheng, M., Drisdell, W. S., Yano, J., Sun, Y. (2015). Bimetal–Organic Framework Self-Adjusted Synthesis of Support-Free Nonprecious Electrocatalysts for Efficient Oxygen Reduction. *ACS Catalysis*, 7068-7076.

Journal Article, Academic Journal (Published)

Jiang, N., You, B., Sheng, M., Sun, Y. (2015). Electrodeposited Cobalt-Phosphorous-Derived Films as Competent Bifunctional Catalysts for Overall Water Splitting. *Angewandte Chemie International Edition*, 54(21), 6251-6254.

Journal Article, Academic Journal (Published)

You, B., Jiang, N., Sheng, M., Bhushan, M. W., Sun, Y. (2015). Hierarchically Porous Urchin-Like Ni₂P Superstructures Supported on Nickel Foam as Efficient Bifunctional Electrocatalysts for Overall Water Splitting. *ACS Catalysis*, 714-721.

Journal Article, Academic Journal (Published)

You, B., Jiang, N., Sheng, M., Gul, S., Yano, J., Sun, Y. (2015). High-Performance Overall Water Splitting Electrocatalysts Derived from Cobalt-Based Metal–Organic Frameworks. *Chemistry of Materials*, 27(22), 7636-7642.

Journal Article, Academic Journal (Published)

Nichols, E. M., Gallagher, J. J., Liu, C., Su, Y., Resasco, J., Yu, Y., Sun, Y., Yang, P., Chang, M. C. Y., Chang, C. J. (2015). Hybrid bioinorganic approach to solar-to-chemical conversion. *Proceedings of the National Academy of Sciences*, 112(37), 11461-11466.

Journal Article, Academic Journal (Published)

You, B., Jiang, N., Sheng, M., Sun, Y. (2015). Microwave vs. solvothermal synthesis of hollow cobalt sulfide nanoprisms for electrocatalytic hydrogen evolution and supercapacitors. *Chemical Communications*, 51(20), 4252-4255.

Journal Article, Academic Journal (Published)

Jiang, N., Bogoev, L., Popova, M., Gul, S., Yano, J., Sun, Y. (2014). Electrodeposited nickel-sulfide films as competent hydrogen evolution catalysts in neutral water. *Journal of Materials Chemistry A*, 2, 19407-19414.