

Published Refereed Journal Articles with Graduate Student Co-authors
Organized by Faculty Mentor
Department of Chemistry and Biochemistry
Publication dates: January 1, 2013 - December 31, 2017

Antony, Edwin

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>

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.

Sorenson, S., Popova, M., Arif, A. M., Berreau, L. (2017). A Bipyridine-ligated Zn(II) Complex with Bridging Flavonolato Ligation: Synthesis, Characterization and Visible Light-induced CO Release Reactivity. *Acta Crystallographica C*, C73, 703-709. doi.org/10.1107/S2053229617011366

Soboleva, T., Esquer, H., Benninghoff, A., Berreau, L. (2017). Sense and release: A thiol-responsive flavonol-based photoCORM that operates via a multiple-input AND logic gate. *Journal of the American Chemical Society*, 139, 9435-9438. pubs.acs.org/doi/abs/10.1021/jacs.7b04077

Popova, M., Soboleva, T., Arif, A. M., Berreau, L. (2017). Properties of a Flavonol-based PhotoCORM in Aqueous Buffered Solutions: Influence of Metal Ions, Surfactants and Proteins on Visible Light-induced CO Release. *RSC Advances*, 7, 21997-22007. pubs.rsc.org/en/content/articlehtml/2017/RA/C7RA02653F

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. *Inorg. Chem.*, 55, 6916-6928. pubs.acs.org/doi/abs/10.1021/acs.inorgchem.6b00456

Anderson, S. N., Larson, M. T., Berreau, L. (2016). Solution or Solid - It Doesn't Matter: Dioxygenase-type Visible Light-induced CO Release Chemistry of Zinc Flavonolato Complexes. *Dalton Trans.*, 45, 14570-14580. pubs.rsc.org/en/content/articlelanding/2016/dt/c6dt01709f#divAbstract

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, 590-594. onlinelibrary.wiley.com/doi/10.1002/open.201500167/abstract

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., 4642-4649.

onlinelibrary.wiley.com/doi/10.1002/ejic.201402254/abstract

Allpress, C. J., Milaczewska, A., Borowski, T., Bennett, J. R., Tierney, D. L., Arif, A. M., Berreau, L. (2014). Halide-promoted Dioxygenolysis of a Carbon-carbon Bond by a Copper(II) Diketonate Complex. *J. Am. Chem. Soc.*, 136, 7821-7824. pubs.acs.org/doi/abs/10.1021/ja502577b

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. www.tandfonline.com/doi/abs/10.1080/00958972.2014.977272?journalCode=gcoo20

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

Allpress, C. J., Berreau, L. (2013). Oxidative Aliphatic Carbon-carbon Bond Cleavage Reactions. *Coord. Chem. Rev.*, 257, 3005-3029. www.sciencedirect.com/science/article/pii/S0010854513001367

Elton, E. S., Zhang, T., Prabhakar, R., Arif, A. M., Berreau, L. (2013). Pb(II)-promoted Amide Cleavage: Mechanistic Comparison to a Zn(II) Analog. *Inorg. Chem.*, 52, 11480-11492. pubs.acs.org/doi/abs/10.1021/ic401782x

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. www.sciencedirect.com/science/article/pii/S0020169313004003

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. pubs.acs.org/doi/abs/10.1021/ja3038189

Boldyrev, Alexander I.

Dong, X., Oganov, A. R., Goncharov, A. F., Stavrou, E., Lobanov, S., Saleh, G., Qian, G.-R., Zhu, Q., Gatti, C., Deringer, V. L., Dronskowski, R., Zhou, X.-F., Prakapenka, V. B., Konopkova, Z., Popov, I. A., Boldyrev, A. I., Wang, H.-T. (2017). A Stable Compound of Helium and Sodium at High Pressure. *Nature Chemistry*, 9, 440-445.

Popov, I. I., Pan, F.-X., You, X.-R., Li, L.-J., Matito, E., Liu, C., Zhai, H.-J., Sun, Z.-M., Boldyrev, A. I. (2016). Peculiar All-Metal σ -Aromaticity of the [Au₂Sb₁₆]⁴⁻ Anion in the Solid State. *55*(49), 15344-15346.

Jian, T., Li, W.-L., Popov, I. A., Lopez, G. V., Chen, X., Boldyrev, A. I., Li, J., Wang, L.-S. (2016). Manganese-Centered Tubular Boron Cluster - MnB₁₆⁻: A New Class of Transition-Metal Molecules. *The Journal of Chemical Physics*, 144(15), 154310.

- Min, X., Popov, I. A., Pan, F.-X., Li, L.-J., Matito, E., Sun, Z.-M., Wang, L.-S., Boldyrev, A. I. (2016). All-Metal Antiaromaticity in Sb₄-Type Lanthanocene Anions. *55*(18), 5531-5535.
- Zhou, X.-F., Oganov, A. R., Wang, Z., Popov, I. A., Boldyrev, A. I., Wang, H.-T. (2016). Two-dimensional magnetic boron. *Physical Review B*, *93*, 085406.
- 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.
- 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.
- Yu, X., Oganov, A. R., Popov, I. A., Boldyrev, A. I. (2016). d-AO Spherical Aromaticity in Ce₆O₈. *Journal Computational Chemistry*, *37*, 103-109.
- 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.
- 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.
- 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.
- 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.
- 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.
- 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.
- 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.
- 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.

- Gish, J. T., Popov, I. A., Boldyrev, A. I. (2015). Homocatenation of Aluminum: Alkane-like Structures of $\text{Li}_2\text{Al}_2\text{H}_6$ and $\text{Li}_3\text{Al}_3\text{H}_8$. *Chemistry - European Journal*, 21(14), 5307–5310.
- Yang, L.-M., Basic, V., Popov, I. A., Boldyrev, A. I., Heine, T., Fraunheim, T., Ganz, E. (2015). Two-dimensional Cu_2Si Monolayer with Planar Hexacoordinate Copper and Silicon Bonding. *Journal of The American Chemical Society*, 137(7), 2757–2762.
- 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} ($\text{M}=\text{S}$ and Se). *Angewandte Chemie International Edition*, 54(5), 1476-1480.
- Minyaev, R. M., Popov, I. A., Koval, V. V., Boldyrev, A. I., Minkin, V. I. (2014). Supertetrahedral B_8O_{20} , C_8O_{20} , and Al_8O_{20} Analogs of Dodecahedrane and their Substituted Molecules. *Structural Chemistry*, 26(1), 223-229.
- 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>
- Ivanov, A., Boldyrev, A. I., Frenking, G. (2014). Inorganic Double-Helix Nanotoroid of Simple Lithium-Phosphorus Species. *Chem. Eur. J.*, 20, 2431-2435.
- 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 CoB_{12}^- and RhB_{12}^- . *J. Phys. Chem. A*.
- 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*.
- 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 B_{24}^- cluster. *J. Chem. Phys.*, 139, 114307.
- Popov, I., Popov, V., Bozhenko, K., Cernusak, I., Boldyrev, A. I. (2013). Structural changes in the series of boron-carbon mixed clusters $\text{C}_x\text{B}_{10-x}^-$ ($x = 3-10$) upon substitution of boron by carbon. *J. Chem. Phys.*, 139, 144307.
- 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-centred aromatic $\text{Ta}@\text{B}_{10}^-$ cluster: Evolution of the Structures of TaB_n^- ($n=3-8$). *J. Chem. Phys.*, 139, 104312.
- 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
- 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.

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.

Olson, J., Boldyrev, A. I. (2013). Planar to 3D Transition in the B6Hy Anions. *J. Phys. Chem. A*, 117, 1614-1620.

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

Chang, Cheng Wei T.

Shrestha, J., Colman, B., Kawasaki, Y., Nziko, V., Subedi, Y., Takemoto, J. Y., Chang, C. W. T. (2017). Synthesis and Bioactivity Investigation of Quinone-based Dimeric Cationic Triazolium Amphiphiles Selective against Resistant Fungal and Bacterial Pathogens. *Eur. J. Med. Chem.*, 126, 596.

Sun, L., Wang, S., Zhang, S., Shao, L., Zhang, Q., Skidmore, C., Chang, C. W. T., Chang, C. W. T., Yu, D., Zhan, J. (2016). Characterization of three tailoring enzymes in dutomycin biosynthesis and generation of a potent antibacterial analogue. *ACS Chemical Biology*, 11, 1992.

Zhang, Q., Alfindee, M., Shrestha, J., Nziko, V., Kawasaki, Y., Peng, X., Takemoto, J., Chang, C. W. T. (2016). Divergent Synthesis of Three Classes of Antifungal Amphiphilic Kanamycin Derivatives. *JOC*, 81, 10651.

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.

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.

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.

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>

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.

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

Dickenson, Nicholas E.

- Burgess, J. L., Burgess, R. A., Morales, Y., Bouvang, J. M., Johnson, S. J., Dickenson, N. (2016). Structural and Biochemical Characterization of Spa7 Provides Mechanistic Insight into Type III Secretion System ATPase Activation and Shigella Virulence Regulation. *Journal of Biological Chemistry*, 291(50), 25837-25852. www.jbc.org/content/early/2016/10/21/jbc.M116.755256.abstract
- Bernard, A. R., Duarte, S., Kumar, P., Dickenson, N. (2016). Detergent isolation stabilizes and activates the Shigella type III secretion system translocator protein IpaC. *Journal of Pharmaceutical Science*, 105(7).

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.

Hengge, Alvan C.

Chu, Y., Williams, N. H., Hengge, A. C. (2017). Transition States and Control of Substrate Preference in the Promiscuous Phosphatase PP1. *Biochemistry*, 56(30), 3923-3933. <http://pubs.acs.org/doi/pdf/10.1021/acs.biochem.7b00441>

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. pubs.acs.org/doi/abs/10.1021/acs.biochem.5b00496

Whittier, S. K., Hengge, A. C., Loria, J. P. (2013). Conformational Motions Regulate Phosphoryl Transfer in Related Protein Tyrosine Phosphatases. *Science*, 341, 899-903. <http://science.sciencemag.org/content/341/6148/899.long>

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

Hevel, Joan M.

Gathiaka, S., Boykin, B., Caceres, T., Hevel, J. M., Acevedo, O. (2016). Understanding protein arginine methyltransferase 1 (PRMT1) product specificity from molecular dynamics. *Bioorg Med Chem*, 24, 4949-4960.

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.

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.

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.

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*.

Johnson, Sean J.

- Burgess, J. L., Burgess, R. A., Morales, Y., Bouvang, J. M., Johnson, S. J., Dickenson, N. (2016). Structural and Biochemical Characterization of Spa7 Provides Mechanistic Insight into Type III Secretion System ATPase Activation and Shigella Virulence Regulation. *Journal of Biological Chemistry*, 291(50), 25837-25852. www.jbc.org/content/early/2016/10/21/jbc.M116.755256.abstract
- 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. academic.oup.com/nar/article/43/3/1848/2411612/Interaction-between-the-RNA-dependent-ATPase-and
- 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. academic.oup.com/nar/article/42/22/13861/2411370/The-Mtr4-ratchet-helix-and-arch-domain-both
- 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*, 533(1-2), 62-68. www.sciencedirect.com/science/article/pii/S0003986113000684
- 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. www.ncbi.nlm.nih.gov/pmc/articles/PMC3557752/
- Johnson, S. J., Jackson, R. N. (2013). Structures of Ski2-like RNA helicases: common themes and complex assemblies. *RNA Biology*, 10(1), 33-43. www.ncbi.nlm.nih.gov/pmc/articles/PMC3590235/

Liu, Tianbiao

- Bo, H., Camden, D., Zayn, R., Liu, T. L. (2017). Long Cycling Neutral Aqueous Redox Flow Batteries towards Sustainable and Safe Energy Storage. *J. Am. Chem. Soc.*
- Shuijian, H., Jian, L., Liu, T. L. (2017). MgCl₂/AlCl₃ Electrolytes for Reversible Mg Deposition/Stripping: Electrochemical Conditioning or not?
- Shuijian, H., Kevin, N., Jian, L., Liu, T. L. (2017). Recent Advances on MgCl₂ Based Electrolytes for Mg Rechargeable Batteries” Energy Storage Mater.

Scheiner, Stephen I.

- Kar, T., Adhikari, U., Scheiner, S. I., Roy, A. K., Parreira, R. L. T., de S. Bergamo, Pedro A., Caramori, G. F., Schneider, F. S. S. (2017). Solvation Enhances the Distinction between Carboxylated Armchair and Zigzag Single-Wall Carbon Nanotubes (SWNT-COOH). *The Journal of Physical Chemistry C*, 121(17), 9516-9527. <http://dx.doi.org/10.1021/acs.jpcc.6b10676>
- Nepal, B., Scheiner, S. I. (2016). Building a Better Halide Receptor. Optimum Choice of Spacer, Binding Unit, and Halosubstitution. *ChemPhysChem*, 17, 836-844.
- Nziko, v., Scheiner, S. I. (2016). Catalysis of the Aza-Diels-Alder Reaction by Hydrogen and Halogen Bonds. *J. Org. Chem.*, 81, 2589-2597.
- 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.
- de Paul N. Nziko, Vincent, Scheiner, S. I. (2016). Effects of Angular Deformation on the Energetics of the SN₂ Reaction. *European Journal of Organic Chemistry*, 2016(23), 3964–3968. <http://dx.doi.org/10.1002/ejoc.201600712>
- Nepal, b., Scheiner, S. I. (2016). Enhancing the Reduction Potential of Quinones via Complex Formation. *J. Org. Chem.*, 81, 4316-4324.
- Kasende, O., nziko, v., Scheiner, S. I. (2016). H-bonding and Stacking Interactions between Chloroquine and Temozolomide. *Int. J. Quantum. Chem.*, 116, 1196-1204.
- Scheiner, S. I. (2016). Highly Selective Halide Receptors Based on Chalcogen, Pnicogen, and Tetrel Bonds. *Chemistry – A European Journal*, 22(52), 18850–18858. <http://dx.doi.org/10.1002/chem.201603891>
- 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>
- Kasende, O. E., Nzuwah-Nziko, Vincent de Paul, Scheiner, S. I. (2016). Interactions between temozolomide and quercetin. *Structural Chemistry*, 27(5), 1577–1588. <http://dx.doi.org/10.1007/s11224-016-0788-8>
- Kasende, O. E., Vincent de Paul N. Nziko, Scheiner, S. I. (2016). Interactions of Nucleic Acid Bases with Temozolomide. Stacked, Perpendicular, and Coplanar Heterodimers. *The Journal of Physical Chemistry B*, 120(35), 9347-9361. <http://dx.doi.org/10.1021/acs.jpcc.6b06150>
- Nepal, b., Scheiner, S. I. (2016). NX··Y Halogen Bonds. Comparison with NH··Y H-bonds and CX··Y Halogen Bonds. *Phys. Chem. Chem. Phys.*, 18, 18015-18023.
- 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.

- 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.
- 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.
- 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>
- Scheiner, S. I. (2015). Dissection of the Factors Affecting Formation of a CH \cdots O H-bond. A Case Study. *Crystals*, 5, 327-345.
- nziko, v. d. P. N., Scheiner, S. I. (2015). Interactions between Thiourea and Imines. Prelude to Catalysis. *J. Org. Chem.*, 54, 10334–10341.
- Nziko, v. d. P. N., Scheiner, S. I. (2015). Intramolecular S \cdots O Chalcogen Bond as Stabilizing Factor in Geometry of Substituted Phenyl-SF₃ Molecules. *J. Org. Chem.*, 80, 2356-2363.
- Nepal, B., Scheiner, S. I. (2015). Long-Range Behavior of Noncovalent Bonds. Neutral and Charged H-Bonds, Pnictogen, Chalcogen, and Halogen Bonds. *Chem. Phys.*, 456, 34-40.
- nepal, b., Scheiner, S. I. (2015). Microsolvation of Anions by Molecules Forming CH \cdots X- Hydrogen Bonds. *Chem. Phys.*, 463, 137-144.
- 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.
- nziko, v., Scheiner, S. I. (2015). S \cdots π Chalcogen Bonds between SF₂ or SF₄ and C-C Multiple Bonds. *J. Phys. Chem. A*, 119, 5889-5897.
- nziko, v., Scheiner, S. I. (2014). Chalcogen Bonding between Tetravalent SF₄ and Amines. *J. Phys. Chem. A*, 118, 10849–10856.
- adhikari, u., Scheiner, S. I. (2014). Competition between Lone Pair- π , Halogen Bond, and Hydrogen Bond in Adducts of Water with Perhalogenated Alkenes C₂Cl_nF_{4-n} (n = 0-4). *Chem. Phys.*, 440, 53-63.
- 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.
- Nepal, B., Scheiner, S. I. (2014). Effect of Ionic Charge upon the CH \cdots π Hydrogen Bond. *J. Phys. Chem. A*, 118, 9575-9587.
- Scheiner, S. I., Adhikari, U. (2014). Effects of Charge and Substituent on the S \cdots N Chalcogen Bond. *J. Phys. Chem. A*, 118, 3183-3192.

- 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.
- Horowitz, S., Dirk, L.M.A., Yesselman, J.D., Nimtz, 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.
- Scheiner, S. I., Adhikari, U. (2013). First Steps in Growth of a Polypeptide Toward β -Sheet Structure. *J. Phys. Chem. B*, 117, 11575-11583.
- Adhikari, U., Scheiner, S. I. (2013). Preferred Configurations of Peptide-Peptide Interactions. *J. Phys. Chem. A*, 117, 489-496.
- 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.
- 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.

Seefeldt, Lance C.

- Davydov, R., Khadka, N., Yang, Z.-Y., Fielding, A. J., Lukoyanov, D., Dean, D. R., Seefeldt, L., Hoffman, B. M. (2016). Exploring electron/proton transfer and conformational changes in the nitrogenase MoFe protein and FeMo-cofactor through cryoreduction/EPR measurements. *Israel Journal of Chemistry*, 56, 841–851. <http://onlinelibrary.wiley.com/doi/10.1002/ijch.201600026/abstract>
- Paengnakorn, P., Ash, P. A., Shaw, S., Danyal, K., Chen, T., Dean, D. R., Seefeldt, L., Vincent, K. A. (2016). Infrared spectroscopy of the nitrogenase MoFe protein under electrochemical control: potential-triggered CO binding. *Chem. Sci.*, (*in press*). <http://pubs.rsc.org/en/Content/ArticleLanding/2016/SC/C6SC02860H>
- Danyal, K., Shaw, S., Page, T. R., Duval, S., Horitani, M., Marts, A. R., Lukoyanov, D., Dean, D. R., Raugei, S., Hoffman, B. M., Seefeldt, L., Antony, E. (2016). Negative cooperativity in the nitrogenase Fe protein electron delivery cycle. *Proceedings of the National Academy of Sciences*, 113, E5783–E5791. <http://www.pnas.org/content/early/2016/09/28/1613089113>
- Khadka, N., Dean, D. R., Smith, D., Hoffman, B. M., Raugei, S., Seefeldt, L. (2016). CO₂ reduction catalyzed by nitrogenase: pathways to formate, carbon monoxide, and methane. *Inorganic Chemistry*, 55(17), 8321–8330. <http://dx.doi.org/10.1021/acs.inorgchem.6b00388>
- Fixen, K. R., Zheng, Y., Harris, D. F., Shaw, S., Yang, Z.-Y., Dean, D. R., Seefeldt, L., Harwood, C. S. (2016). Light-driven carbon dioxide reduction to methane by nitrogenase in a photosynthetic bacterium. *Proceedings of the National Academy of Sciences*, 113(36), 10163–10167. <http://www.pnas.org/content/113/36/10163>

- Milton, R. D., Abdellaoui, S., Khadka, N., Dean, D. R., Leech, D., Seefeldt, L., Minter, S. D. (2016). Nitrogenase bioelectrocatalysis: heterogeneous ammonia and hydrogen production by MoFe protein. *Energy & Environmental Science*, 9(8), 2550–2554.
<http://pubs.rsc.org/en/content/articlelanding/2016/ee/c6ee01432a>
- Lukoyanov, D., Khadka, N., Yang, Z.-Y., Dean, D. R., Seefeldt, L., Hoffman, B. M. (2016). Reductive elimination of H₂ activates nitrogenase to reduce the N≡N triple bond: characterization of the E4(4H) Janus intermediate in wild-type enzyme. *Journal of the American Chemical Society*, 138(33), 10674–10683.
<http://dx.doi.org/10.1021/jacs.6b06362>
- Yang, Z.-Y., Ledbetter, R., Shaw, S., Pence, N., Tokmina-Lukaszewska, M., Eilers, B., Guo, Q., Pokhrel, N., Cash, V. L., Dean, D. R., Antony, E., Bothner, B., Peters, J. W., Seefeldt, L. (2016). Evidence that the Pi release event is the rate-limiting step in the nitrogenase catalytic cycle. *Biochemistry*, 55, 3625–3635.
<http://dx.doi.org/10.1021/acs.biochem.6b00421>
- Brown, K. A., Harris, D. F., Wilker, M. B., Rasmussen, A., Khadka, N., Hamby, H., Keable, S., Dukovic, G., Peters, J. W., Seefeldt, L., King, P. W. (2016). Light-driven dinitrogen reduction catalyzed by a CdS:nitrogenase MoFe protein biohybrid. *Science*, 352(6284), 448–450.
<http://science.sciencemag.org/content/352/6284/448>
- Lukoyanov, D., Khadka, N., Yang, Z.-Y., Dean, D. R., Seefeldt, L., Hoffman, B. M. (2016). Reversible photoinduced reductive elimination of H₂ from the nitrogenase dihydride state, the E4(4H) Janus intermediate. *Journal of the American Chemical Society*, 138(4), 1320–1327.
<http://pubsdc3.acs.org/doi/full/10.1021/jacs.5b11650>
- 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>
- 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. *Bioresour Technol*, 196, 431–440.
<http://www.sciencedirect.com/science/article/pii/S0960852415010391>
- 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>
- McCurdy, A. T., Higham, A. J., Morgan, M. R., Quinn, J., Seefeldt, L. (2014). Two-step process for production of biodiesel blends from oleaginous yeast and microalgae. *Fuel*, 137, 269–276.
<http://www.sciencedirect.com/science/article/pii/S0016236114007649>
- Willis, R. M., McCurdy, A. T., Ogborn, M. K., Wahlen, B. D., Quinn, J., Pease, III, L. F., Seefeldt, L. (2014). Improving energetics of triacylglyceride extraction from wet oleaginous microbes. *Bioresour Technol*, 167, 416–424.
<http://www.sciencedirect.com/science/article/pii/S0960852414008578>

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

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.

Sun, Yujie

You, B., Liu, X., Jiang, N., Sun, Y. (2016). A General Strategy for Decoupled Hydrogen Production from Water Splitting by Integrating Oxidative Biomass Valorization. *Journal of the American Chemical Society*, 138(41), 13639-13646.

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.

Jiang, N., You, B., Boonstra, R., Terrero Rodriguez, I. M., Sun, Y. (2016). Integrating Electrocatalytic 5-Hydroxymethylfurfural Oxidation and Hydrogen Production via Co–P-Derived Electrocatalysts. *ACS Energy Letters*, 386-390.

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

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.

You, B., Jiang, N., Liu, X., Sun, Y. (2016). Simultaneous H₂ Generation and Biomass Upgrading in Water by an Efficient Noble-Metal-Free Bifunctional Electrocatalyst. *Angewandte Chemie International Edition*, 55(34), 9913-9917.

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.

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.

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.

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.

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.

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.

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.