

## Publications – 2017

### A. Journal Articles

1. Deria, P.; Yu, J.; Tanner, S.; Balaraman, R. P. Ground-State versus Excited-State Interchromophoric Interaction: Topology Dependent Excimer Contribution in Metal–Organic Framework Photophysics. *J. Am. Chem. Soc.* 2017, 139, 5973-5983.
2. Hartlied, K. J.; Peters, A. W.; Wang, T. C.; Deria, P.; Farha, O. K.; Hupp, J. T.; Stoddart, J. F. Functionalised cyclodextrin-based metal–organic frameworks. *Chem. Commun.* 2017, 53, 7561-7564.
3. Zhu J, Huang X, Du Z. Widespread Occurrence of CPK-1 Pseudoknots and Related RNA Structures. *Research Journal of Life Sciences, Bioinformatics, Pharmaceutical and Chemical Sciences*, 3(1):1-16 (2017).
4. Tang, M. & Ge, Q. Mechanistic Understanding on Oxygen Evolution Reaction on  $\gamma$ -FeOOH (010) in Alkaline Solution Based on DFT Computational Study, *Chin. J. Catal.* 38, 1621-1628 (2017).
5. Ye, J.; Zhang, T.; Xu, L.; Yin, S.; Weerasinghe, K.; Ubaldo, P.; He, P. & Ge. Q. Surface Chemical Properties of Mo<sub>2</sub>C, W<sub>2</sub>C, Mo<sub>2</sub>N and W<sub>2</sub>N Probed with CO, CO<sub>2</sub> and O<sub>2</sub> Adsorption: A DFT Analysis, *J. Electrochemistry (China)*, 23, 371-380 (2017).
6. Zhai, L.; Cui, C.; Zhao, Y.; Zhu, X.; Han, J.; Wang, H. & Ge Q. Titania-Modified Ag Electrocatalyst for Selective CO<sub>2</sub> Reduction to CH<sub>3</sub>OH and CH<sub>4</sub> from DFT Study, *J. Phys. Chem. C*, 121, 16275-16282 (2017).
7. Wang, X.; Ding, S.; Wang, H.; Liu, X.; Han, J.; Ge, Q. & Zhu, X. Conversion of propionic acid and 3-pentanone to hydrocarbons on ZSM-5 catalysts: reaction pathway and active site, *Appl. Catal. A*. 545, 79-89 (2017).
8. Ding, S.; Ge, Q. & Zhu, X. Research Progress in Ketonization of Biomass-derived Carboxylic Acids over Metal Oxides *Acta Chim. Sinica*, 75, 439-447 (2017).
9. Rui, N.; Wang, Z.; Sun, K.; Ye, J.; Ge, Q. & Liu, C.-j. CO<sub>2</sub> hydrogenation to methanol over Pd/In<sub>2</sub>O<sub>3</sub>: effects of Pd and oxygen vacancy, *Appl. Catal. B*, 218, 488-97 (2017).
10. Liu, D.; Li, G.; Yang, F.; Wang, H.; Han, J.; Zhu, X. & Ge, Q. Competition and Cooperation of Hydrogenation and Deoxygenation Reactions during Hydrodeoxygenation of Phenol on Pt(111), *J. Phys. Chem. C*, 121, 12249–12260 (2017).
11. Sun, J.; Wang, H.; Gao, X.; Zhu, X.; Ge, Q.; Liu, X. & Han J. Mesoporous silica-based nanotubes loaded Pd nanoparticles: Effect of framework compositions on the performance in heterogeneous catalysis, *Microporous and Mesoporous Mater.* 247, 1-8 (2017).
12. Yang, F.; Liu, D.; Wang, H.; Liu, X.; Han, J.; Ge, Q. & Zhu, X. Geometric and electronic effects of bimetallic Ni-Re catalysts for selective deoxygenation of m-cresol to toluene, *J. Catal.* 349, 84-97 (2017).
13. “NMR Hyperpolarization Techniques of Gases.” Danila A. Barskiy, Aaron M. Coffey, Panayiotis Nikolaou, Dmitry M. Mikhaylov, Boyd M. Goodson, Rosa T. Branca, George J. Lu, Mikhail G. Shapiro, Ville-Veikko Telkki, Vladimir V. Zhivonitko, Igor V. Koptuyug, Oleg G. Salnikov, Kirill V. Kovtunov, Valerii I. Bukhtiyarov, Matthew S. Rosen, Michael J. Barlow, Shahideh Safavi, Ian P. Hall, Leif Schroder, and Eduard Y. Chekmenev. contributed cover article / “mini-review” for *Chem. Eur. J.*, published online DOI: 10.1002/chem.201603884, December 5 (2016); final print: 23, 725-751 (2017) (with frontispiece published on p. 724).
14. “Robust Imidazole-<sup>15</sup>N<sub>2</sub> Synthesis for High-Resolution Low-Field (0.05 T) 15N Hyperpolarized NMR Spectroscopy.” R.V. Shchepin, D.A. Barskiy, A.M. Coffey, M.A. Feldman, L.M. Kovtunova, V.I. Bukhtiyarov, K.V. Kovtunov, B.M. Goodson, I.V. Koptuyug, E.Y. Chekmenev, *Chemistry Select.* 2, 4478 – 4483 (2017).
15. “The Absence of Quadrupolar Nuclei Facilitates Efficient <sup>13</sup>C Hyperpolarization via Reversible Exchange with Parahydrogen.” Danila A. Barskiy, Roman V. Shchepin, Christian P. N. Tanner,

- Johannes F. P. Colell, Boyd M. Goodson, Thomas Theis, Warren S. Warren, and Eduard Y. Chekmenev. *ChemPhysChem*, 18, 1493 – 1498 (2017).
16. "Toward Hyperpolarized  $^{19}\text{F}$  Molecular Imaging via Reversible Exchange with Parahydrogen." Roman V. Shchepin, Boyd M. Goodson, Thomas Theis, Warren S. Warren, and Eduard Y. Chekmenev. *ChemPhysChem*, DOI: 10.1002/cphc.201700594 Published online May 29. 18, 1961 – 1965 (2017).
  17. "Aqueous, Heterogeneous Parahydrogen-Induced  $^{15}\text{N}$  Polarization." Liana B. Bales, Kirill V. Kovtunov, Danila A. Barskiy, Roman V. Shchepin, Aaron M. Coffey, Larisa M. Kovtunova, Andrey V. Bukhtiyarov, Matthew Feldman, Valerii I. Bukhtiyarov, Eduard Y. Chekmenev, Igor V. Koptuyug, and Boyd M. Goodson. *J. Phys. Chem. C*, DOI: 10.1021/acs.jpcc.7b05912, published online June 21, 121, 15304–15309 (2017).
  18. "Heterogeneous Microtesla SABRE Enhancement of  $^{15}\text{N}$  NMR Signals." Kirill V. Kovtunov, Larisa M. Kovtunova, Max E. Gemeinhardt, Andrey V. Bukhtiyarov, Jonathan Gesiorski, Valerii I. Bukhtiyarov, Eduard Y. Chekmenev, Igor V. Koptuyug, Boyd M. Goodson. *Angew. Chem. Intl. Ed.*, DOI: 10.1002/anie.201705014, published online June 23, 56, 10433 –10437 (2017).
  19. "Imaging of Biomolecular NMR Signals Amplified by Reversible Exchange with Parahydrogen Inside an MRI Scanner." K.V. Kovtunov, B.E. Kidd, O.G. Salnikov, L.B. Bales, M.E. Gemeinhardt, J. Gesiorski, R.V. Shchepin, E.Y. Chekmenev, B.M. Goodson, I.V. Koptuyug. *J. Phys. Chem. C* 121, 25994–25999 (2017).
  20. "Spin Relays Enable Efficient Long-Range Heteronuclear Signal Amplification by Reversible Exchange." R.V. Shchepin, L. Jaigirdar, T. Theis, W.S. Warren, B.M. Goodson, E.Y. Chekmenev. *J. Phys. Chem. C*, 121, 28425–28434 (2017).
  21. Pradeep Ramiah Rajasekaran, Chuanhong Zhou, Mallika Dasari Reddy, Kay-Obbe-Voss, Christina Trautmann, and Punit Kohli "Polymeric Lithography Editor: Editing Lithographic Errors with Nanoporous Polymeric Probes", *Science Advances* 2017; 3: e1602071 9 June 2017 (highlight at the University of Maryland press release, twitter (<https://twitter.com/ScienceAdvances/status/875007362255507457>), and the rotating banner at <http://advances.sciencemag.org/>).
  22. Rajiv Dhital, Nathalie Becerra Mora, Prabesh Joshi, Arosha Umagiliyage, Tan Chai, Derek Fisher, Punit Kohli, Ruplal Choudhary "Integrity of edible Nano-coatings and its effects on quality of strawberries subjected to simulated in-transit vibrations" *LWT- Food Science and Technology* 2017, 80, 257-264.
  23. Jasmyn S Abrams, Savannah E Howe, Nathalie Becerra, Punit Kohli, Vjollca Konjufca. "Immunogenicity of Antigen-Conjugated Biodegradable Polydiacetylene Liposomes Administered Mucosally" *Journal of Biomedical Materials Research Part A* 2017, 105, 557-565.
  24. Arosha Loku Umagiliyage, Nathalie Becerra-Mora, Punit Kohli, Derek J Fisher, Ruplal Choudhary "Antimicrobial efficacy of liposomes containing d-limonene and its effect on the storage life of blueberries" *Postharvest Biology and Technology* 2017, 128, 130-137.
  25. "Examining the Craft Brew Industry: Identifying Research Needs", Sylvia Smith, John Farrish, Matthew McCarroll and Elizabeth Huseman, *International Journal of Hospitality Beverage Management*, vol 1, Number 1, Article 3, 1-17, 2017 (Inaugural Issue).
  26. Bheemireddy, S., Hautzinger, M.P., Li, T., Lee, B., Plunkett, K.N.\*, "Conjugated Ladder Polymers by a Cyclopentannulation Polymerization", *J. Am. Chem. Soc.*, 2017, 139, 5801-5807.
  27. Shao, B., Zhu, X., Plunkett, K.N.\*, Vanden Bout, D.A.\*, "Controlling the Folding of Conjugated Polymers at the Single Molecule Level via Hydrogen Bonding", *Polym. Chem.* 2017, 8, 1188-1195.
  28. Chen, S. and Shamsi, M. H.\* (2017) Biosensors-on-Chip: A Tropical Review. *Journal of Micromechanics and Microengineering*, 27, 083001 (15pp) (Invited review).

29. Léon, J. C., She, Z., Kamal, A., Shamsi, M. H., Müller, J., Kraatz, H.-B. (2017) DNA Films Containing the Artificial Nucleobase Imidazole Mediate Charge Transfer in a Silver(I)-Responsive Way. *Angewandte Chemie International Edition*, 56, 1-6.
30. She, Z., Topping, K., Dong, B., Shamsi, M. H. and Kraatz, H.-B. (2017) An Unexpected Use of Ferrocene: A Scanning Electrochemical Microscopy Study of A Toll-Like Receptor Array and its Interaction with E. Coli. *Chemical Communication*, 53, 2946-2949.
31. Li Fan and Ian I. Suni, J. *Electrochem. Soc.* 164 (2017), D681-D686: "Electrodeposition and Capacitance Measurements of WS<sub>2</sub> Thin Films."
32. Bamidele D. Falola, Li Fan, Tomasz Wiltowski and Ian I. Suni, J. *Electrochem. Soc.* 164 (2017), D674-D679: "Electrodeposition of Cu-doped MoS<sub>2</sub> for Charge Storage in Electrochemical Supercapacitors."
33. Madhavi Pali, James E. Garvey, Brian C. Small and Ian I. Suni, *Sens. Biosens. Res.* 13 (2017), 1-8: "Impedance Detection of Fish Hormones by Electrochemical Impedance Spectroscopy and Quartz Crystal Microbalance,"
34. Bei Miao, Zhipeng Wu, Han Xu, Minhua Zhang, Yifei Chen, Lichang Wang, *Chem. Phys. Lett.* 688(2017)92-97: "Ir catalysts: Preventing CH<sub>3</sub>COOH formation in ethanol oxidation".
35. Han Xu, Bei Miao, Minhua Zhang, Yifei Chen, Lichang Wang, *Phys. Chem. Chem. Phys.* 19(2017)26210-26220: "Mechanism of C-C and C-H bond cleavage in ethanol oxidation reaction on Cu<sub>2</sub>O(111): A DFT-D and DFT+U study".
36. Zhipeng Wu, Minhua Zhang, Haoxi Jiang, Chuan-Jian Zhong, Yifei Chen, Lichang Wang, *Phys. Chem. Chem. Phys.* 19(2017)15444-15453: "Competitive C-C and C-H bond scission in the ethanol oxidation reaction on Cu(100) and the effect of an alkaline environment".
37. Tianyang Wang, Krishanthi C. Weerasinghe, Haiya Sun, Ping'an Li, Dongzhi Liu, Wei Li, Wenping Hu, Xueqin Zhou, Lichang Wang, *J. Mol. Struct.* 1142(2017)226-238: "Characterization of photo-induced electron and hole transfer in a porphyrin based ambipolar organic molecule with cascade energy levels".
38. Ruitao Wu, Lichang Wang, *Chem. Phys. Lett.* 678(2017)196-202: "Alloying effect via comparative studies of ethanol dehydrogenation on Cu(111), Cu<sub>3</sub>Pd(111), and Cu<sub>3</sub>Pt(111)".
39. Haiya Sun, Dongzhi Liu, Tianyang Wang, Ting Lu, Wei Li, Siyao Ren, Wenping Hu, Lichang Wang, Xueqin Zhou, *ACS Appl. Mater. Interfaces* 9(2017)9880-9891: "Enhanced Internal Quantum Efficiency in Dye-Sensitized Solar Cells: Effect of Long-Lived Charged-Separated State of Sensitizers".
40. Xiaoyun Fan, Zhipeng Wu, Lichang Wang, Chuanyi Wang, *Chem. Mater.* 29(2017)639-647: "Exploring the Origin of High Dechlorination Activity in Polar Materials M<sub>2</sub>B<sub>5</sub>O<sub>9</sub>Cl (M= Ca, Sr, Ba, Pb) with Built-in Electric Field".
41. Tianyang Wang, Haiya Sun, Linli Zhang, Nathan D. Colley, Chelsea N. Bridgmohan, Dongzhi Liu, Wenping Hu, Wei Li, Xueqin Zhou, Lichang Wang, *Dyes Pigm.* 139(2017)601-610: "Effect of photo-induced charge separated state lifetimes in donor-acceptor1-acceptor2 organic ambipolar semiconductors on their photovoltaic performances".
42. Tianyang Wang, Haiya Sun, Ting Lu, Chelsea N. Bridgmohan, Fengqing Li, Dongzhi Liu, Wenping Hu, Wei Li, Xueqin Zhou, Lichang Wang, *Dyes Pigm.* 139(2017)264-273: "Dissociation exists in s-triazine based donor-acceptor organic systems by photo-induced electron transfer".
43. Chuanwu Zhao, Tianyang Wang, Dongmei Li, Ting Lu, Dongzhi Liu, Qingbo Meng, Qianqian Zhang, Fengqing Li, Wei Li, Wenping Hu, Lichang Wang, Xueqin Zhou, *Dyes Pigm.* 137(2017)256-265: "Synthesis and characterization of triphenylamine modified azobenzene dyes".
44. Krishanthi C. Weerasinghe, Tianyang Wang, Junpeng Zhuang, Dongzhi Liu, Wei Li, Xueqin Zhou, and Lichang Wang, *Comput. Mater. Sci.* 126(2017)244-251: "Mechanistic study and design of porphyrin derivatives for inducing the triplet state of perelene bismide".

45. Ting Lu, Haiya Sun, Nathan D. Colley, Chelsea N. Bridgmohan, Dongzhi Liu, Wei Li, Wenping Hu, Xueqin Zhou, Tianyang Wang, and Lichang Wang, *Dyes Pigm.* 136(2017)404-415: “Tuning the donors to control the lifetimes of charge separated states in triazine-based Donor-Acceptor systems”.

#### B. Books & Book Chapters

1. Rohilla, K.J., and Gagnon, K.T. (2017) RNA Biology of Disease-Associated Microsatellite Repeat Expansions. *Acta Neuropath. Comm.*, 5:63.
2. “The Physics of Hyperpolarized Gas MRI.” Boyd M. Goodson, Kaili Ranta, Jason Skinner, Aaron M. Coffey, Peter Nikolaou, Max Gemeinhardt, Drake Anthony, Shawn Stephenson, Steven Hardy, John Owers-Bradley, Michael J. Barlow, and Eduard Y. 32 Chekmenev, invited chapter for: *Hyperpolarized and Inert Gas MRI From Technology to Application in Research and Medicine* (peer-reviewed); Mitchell Albert and Francis Hane (Eds.), Academic Press / Elsevier (London); ISBN: 978-0-12-803675-4; pp 23-40 (2017).
3. “Using Raman Spectroscopy to Improve Hyperpolarized Noble Gas Production for Clinical Lung Imaging Techniques.” Jonathan Birchall, Nicholas Whiting, Jason Skinner, Michael J. Barlow and Boyd M. Goodson, In: *Raman Spectroscopy and Applications*, Dr. Khan Maaz (Ed.), InTech, DOI: 10.5772/65114. Published online February 15 (2017).

#### C. Patents

1. “pH-Sensitive Imaging Agents.” Yong Gao, Boyd Goodson, Patent # US 9,682,157 B2, (June 20, 2017).
2. “Heterogeneous Catalysts for NMR/MRI Enhancement via signal amplification by reversible exchange (SABRE)” Chekmenev, E.Y., Goodson, B.M., Milton, T.L., Shi, F. Patent # US 9,707,550 B2, (July 18, 2017).
3. “Water soluble catalysts for NMR/MRI enhancement” Chekmenev, E.Y., Goodson, B.M., Milton, T.L., He, P., Best, Q.A., Shi, F., Groome, K.A., Patent # US 9,790,245 B2 (Oct. 17, 2017).