List of publication of Dr. Djamaladdin (Jamal) G. Musaev

Director, Cherry L. Emerson Center for Scientific Computation,
Emory University, Atlanta, GA, 30322

2022

1. David M. Soro, Jose B. Roque, Jonas W. Rackl, Bohyun Park, Stefan Payer, Yuan Shi, J. Craig Ruble, Mu-Hyun Baik, Djamaladdin G. Musaev, Richmond Sarpong "Photo- and Metal-Mediated Deconstructive Approaches to Cyclic Aliphatic Amine Diversification", **2022**, *submitted*

2. Zihao Xu, Bingya Hou, Fengyi Zhao, Yawei Liu, Haotian Shi, Zhi Cai, Yurui Mu, Craig L. Hill, Djamaladdin G. Musaev, Stephen Cronin, Tianquan Lian, "*In situ* Transient Spectroscopic Probe of Key Loss Pathways in GaP/TiO_2 Photocathodes for Solar Hydrogen Generation", **2022**, *submitted*

3. Li-Ping Xu, Shaoqun Qian, Zhe Zhuang, Jin-Quan Yu, Djamaladdin G. Musaev, "Unconventional Mechanism and Selectivity of the Pd-Catalyzed C–H Bond Lactonization in Aromatic Carboxylic Acid", *Nature Comm.* **2022**, *13, 1-8*

4. Li-Ping Xu, Zhe Zhuang, Shaoqun Qian, Jin-Quan Yu, Djamaladdin G. Musaev, "Roles of Ligand and Oxidant in the Pd(II)-Catalyzed and Ligand-enabled C(sp^3)–H Lactonization in Aliphatic Carboxylic Acid: The Mechanistic Studies." *ACS Catalysis,* **2022**, *12,* 4848-4858

5. Li-Ping Xu, Adrian Varela-Alvarez, and Djamaladdin G. Musaev, "(Tetracarboxylate)bridged-di-Transition Metal Complexes and Factors Impacting to Their Carbene Transfer Reactivity", In the book "*Catalysis for a Sustainable Environment* "; Edited by A. Pombeiro and coworkers., **2022**, pp.@@, *accepted*

6. Alexey L. Kaledin, Jose B. Roque, Richmond Sarpong, Djamaladdin G. Musaev, "Computational Study of Key Mechanistic Details for a Proposed Copper(I)-Mediated Deconstructive Fluorination of *N*-Protected Cyclic Amines", *Topics in Catal.,* **2022**, *65(1),* 418-432

7. Meilin Tao, Qiushi Yin, Alexey, L. Kaledin, Natalie Uhlikova, Xinlin Lu, Ting Cheng, Yu-Sheng Chen, Tianquan Lian, Yurii V. Geletii, Djamaladdin G. Musaev, John Bacsa, Craig L. Hill, "Structurally precise two-transition-metal water oxidation catalysts. Quantifying adjacent 3d metals by synchrotron X-radiation anomalous dispersion scattering." *Inorg. Chem.*, **2022**, *61(16)*, 6252 - 6262

8. R. Nallagonda, Djamaladdin G. Musaev, R. R. Karimov, "Light-Promoted Dearomative cross-coupling of heteroarenium salts and aryl iodides via Nickel catalysis," *ACS Catalysis,* **2022***,* 12, 1818-1829.

2021

9. Charis Amber Roberts, Bohyun Park, Li-Ping Xu, Jose B. Roque, Charles S. Yeung, Djamaladdin G. Musaev, Richmond Sarpong, Rebecca Lyn LaLonde, "Sequential Norrish-Yang Cyclization and C–C Cleavage/Cross-Coupling of a [4.1.0] Fused Saturated Azacycle", *J. Org. Chem.,* **2021**, *86* (17), 12436-12442

10. Zihao Xu, Bingya Hou, Fengyi Zhao, Zhi Cai, Haotian Shi, Yawei Liu, Craig L. Hill, Djamaladdin G. Musaev, Stephen B. Cronin, Tianquan Lian, "Nanoscale TiO_2 Protection Layer Enhances the Built-in Field and Charge Separation Performance of GaP Photoelectrodes." *Nano Lett*, **2021**, *21 (19)*, 8017-8024

11. Q. Yin, Yurii V. Geletii, Tianquan Lian, Djamaladdin G. Musaev, Craig L. Hill, "Polyoxometalate Systems to Probe Catalyst Environment and Structure in Water Oxidation Catalysis," *Adv. in Inorganic Chem.*, **2021**, v. 79, ch. 10, pp. @@, *accepted*

12. Torben Rogge, Nikolaos Kaplaneris, Naoto Chatani, Jinwoo Kim, Sukbok Chang, Benudhar Punji, Laurel L. Schafer, Djamaladdin G. Musaev, Joanna Wencel-Delord, Charis A. Roberts, Richmond Sarpong, Zoe E. Wilson, Margaret A. Brimble, Magnus J. Johansson, Lutz Ackermann, „C–H Activation", *Nature Reviews Methods Primers*, **2021**, 1 (1), 1-31

13. Alexey L. Kaledin, Tianquan Lian, Craig L. Hill, Djamaladdin G. Musaev, "An All-Atom Theory of Electron Transfer at Nanocrystal/Molecule Interfaces: A Hybrid LCAO/DFT Approach", *J. Phys. Chem. C*, **2021**, *125 (9)*, 5116-5126.: doi: 10.1021/acs.jpcc.0c11572

14. Aaron G. Nash, Colton J. Breyer, Brett D. Vincenzini, Gregory I. Elliott, Jens Niklas, Oleg G. Poluektov, Arnold L. Rheingold, Diane K. Smith, Djamaladdin G. Musaev, Douglas B. Grotjahn, „ A Water Oxidation Catalyst with a Sulfonate Moiety in the Ruthenium Active Site is Highly Active in both Neutral and Acidic Media", *Angew. Chem. Int. Ed.* **2021**, *60*, 1540–1545: doi.org/10.1002/anie.202008896

15. Daniel L. Collins-Wildman, Kevin P. Sullivan, Yurii V. Geletii, Wesley O. Gordon, Alex Balboa, Yiyao Tian, Alexey L. Kaledin, Rachel M. Slaugenhaupt, Victoria G. Snider, Christopher J. Karwacki, Anatoly I. Frenkel, Djamaladdin G. Musaev, Craig L. Hill, „ A Solvent-Free Solid Catalyst for the Selective and Color-Indicating Ambient-Air Removal of Sulfur Mustard", *Commun. Chem,* **2021**, *4,* 33: https://doi.org/10.1038/s42004-021-00465-7

16. Brandon E. Haines, Djamaladdin G. Musaev, "Hydrogen-Bonding as a Factor to Determine the Regioselectivity for Pd-mediated C−H Activation of Pyridine", *ChemCatChem*, **2021**, 13(4), 1201-1206: https://doi.org/10.1002/cctc.202001658

17. Anna R. Kaplan, Djamaladdin G. Musaev, William M. Wuest, "Pyochelin Biosynthetic Metabolites Bind Iron and Promote Growth in *Pseudomonads* Demonstrating Siderophore-like Activity"*ACS Infect. Dis.* **2021**, *7, 3,* 544–551

18. Zhi Ren, Djamaladdin G. Musaev, Huw M. L. Davies, "Influence of Aryl Substituents on the alignment of ligands in the Dirhodium Tetrakis(1,2,2-Triarylcyclopropanecarboxylate) Catalysts", *ChemCatChem*, **2021,** *13*, 174 –179: *doi.org/10.1002/cctc.202001206*

19. Qiushi Yin, Zihao Xu, Tianquan Lian, Djamaladdin G. Musaev, Craig L. Hill, Yurii V. Geletii, "Tafel Slope Analyses for Homogeneous Catalytic Reactions", *Catalysts* **2021**, *11*(1), 87; https://doi.org/10.3390/catal11010087

20. Jose B. Rogue, Richmond Sarpong, Djamaladdin G. Musaev, "Key Mechanistic Features of the Silver(I)-Mediated Deconstructive Fluorination of Cyclic Amines: Multistate Reactivity versus Single-Electron Transfer**"** *J. Am. Chem. Soc.* **2021**, *143, 10,* 3889–3900**:** https://doi.org/10.1021/jacs.0c13061

21. Deston R. Lian, Lanny S. Liebeskind, Djamaladdin G. Musaev, "Mechanistic details of the dehydrative carbon-heteroatom bond construction viathe benzoisochalcogenazolone-catalyzed acylative oxidation−reduction−condensation strategy", *ARVIKOC,* **2021**, 3.

22. Yiyao Tian, Alexey L. Kaledin, Daniel L. Collins-Wildman, Djamaladdin G. Musaev, Craig L. Hill, Anatoly I. Frenkel, "Probing Atomic-level details of Nerve Agent Adsorption and Decomposition over One-Dimensional Polyniobates", *ACS Applied Nano Materials,* **2021**, 21, 4, 6, 5649–5654.

2020

23. LiPing Xu, Jose B. Rogue, Richmond Sarpong, Djamaladdin G. Musaev, „Reactivity and Selectivity Controlling factors in the Pd/diakylbiarylphosphine-catalyzed C–C cleavage/cross-coupling of an *N*-fused bicyclo α-hydroxy-β-lactam“, *J. Am. Chem. Soc*., **2020**, 142, 50, 21140–21152: https://doi.org/10.1021/jacs.0c10220

24. Zihao Xu, Yiming Huang, Yulei Cao, Tao Jin, Kristen A. Miller, Alexey L. Kaledin, Djamaladdin G. Musaev, Tianquan Lian, Eilaf Egap, "Enhanced Intersystem Crossing of Boron Dipyrromethene by TEMPO Radical", *JCP*, **2020**, *153 (15)*, 154201: https://doi.org/10.1063/5.0025972

25. Chase A. Salazar, Kaylin N. Flesch, Brandon E. Haines, Philip S. Zhou, Djamaladdin G. Musaev, Shannon S. Stahl, "Palladium-catalyzed C–H oxidative arylation accessing high turnover with O2*", Science*, **2020**, 370 (6523), 1454-1460: DOI: 10.1126/science.abd1085

26. David L. Bruns, Djamaladdin G. Musaev, Shannon S. Stahl, „Insights into Ligand Effects on Palladium(II) Reduction Potentials Accessed via Palladium(II)/Hydroquinone Redox Equilibria“, *J. Am. Chem. Soc.* **2020**, *142 (46),* 19678-19688: https://doi.org/10.1021/jacs.0c09464

27. Alexey L. Kaledin, Qiushi Yin, Craig L. Hill, Timquan Lian, Djamaladdin G. Musaev, „Ion-Pairing in Polyoxometalate Chemistry: Impact of Fully Hydrated Alkali Metal Cations on Properties of the Keggin $[PW_{12}O_{40}]^{3-}$ Anion“, *Dalton Trans*, **2020**, *49 (32),* 11170-11178. Doi: 10.1039/D0DT02239J

28. Benjamin Wertz, Zhi Ren, John Bacsa, Djamaladdin G. Musaev, Huw M. L. Davies, „Comparison of 1,2-Diarylcyclopropanecarboxylates with 1,2,2-Triarylcyclopropanecarboxylates as chairal ligands for dirhodium-catalyzed cyclopropanation and C-H functionalization“, *J. Org. Chem.*, **2020**, *85 (19),* 12199-12211: https://doi.org/10.1021/acs.joc.0c01276

29. Li-Ping Xu, Elaine E. L.-N. Liu, John Bacsa, Cora E. MacBeth, and Djamaladdin G. Musaev, "Mechanistic Details of the Cobalt-Mediated Dehydrogenative Dimerization of Aminoquinoline-Directed Benzamides", *Chem Sci*., **2020**, *11*, 6085-6096.

30. Maizie Lee, Zhi Ren, Djamaladdin G. Musaev, Huw M. L. Davies, „Rhodium-Stabilized Diarylcarbenes behaving as Donor/Acceptor Carbenes“, *ACS Catalysis*, **2020**, *10*, 6240-6247.

31. Tyler G. Grissom, Anna M. Plonka, Conor H. Sharp, Amani M. Ebrahim, Yiyao Tian, Daniel L. Collins-Wildman, Alexey L. Kaledin, Diego Troya, Craig L. Hill, Anatoly I. Frenkel, Djamaladdin G. Musaev, Wesley O. Gordon, Chris J. Karwacki, Mark B. Mitchell, John R. Morris, „Metal-Organic Framework- and Polyoxometalate-Based Sorbents for the Uptake and Destruction of Chemical Warfare Agents“, *ACS Applied Materials & Interfaces*, **2020**, *12 (13),* 14641-14661

32. Li-Ping Xu, Brandon E. Haines, Manjaly J. Ajitha, Kei Murakami, Kenichiro Itami, Djamaladdin G. Musaev, "Roles of Base in the Pd-Catalyzed Annulative Chlorophenylene Dimerization", *ACS Catalysis*, **2020**, *10*, 3059-3073.

33. Jose B. Roque, Yusuke Kuroda, Justin Jurczyk, Li-Ping Xu, Jin Su Ham, Lucas T. Göttemann, Charis A. Roberts, Donovon Adpressa, Josep Saurí, Leo A. Joyce, Djamaladdin G. Musaev, Charles S. Yeung, Richmond Sarpong, "C−C Cleavage Approach to C−H Functionalization of Saturated Aza-Cycles", *ACS Catalysis*, **2020**, *10*, 2929-2941.

2019

34. Alexey L. Kaledin, Craig L. Hill, Tianquan Lian, Djamaladdin G. Musaev, „A Bulk Adjusted Linear Combination of Atomic Orbitals (BA-LCAO) Approach for Nanoparticles“, *J. Comput. Chem.* **2019**, *40(1)*, 212-221

35. Amani M. Ebrahim, Anna M. Plonka, Yiyao Tian, Sanjaya D. Senanayake, Wesley O. Gordon, Alex Balboa, Hui Wang, Daniel L. Collins Wildman, Craig L. Hill, Djamaladdin G. Musaev, John

R. Morris, Diego Troya, Anatoly I. Frenkel, „Multimodal Characterization of Materials and Decontamination Processes for Chemical Warfare Protection“, *ACS Applied Materials & Interfaces*, **2019**, 12 (13), 14721-14738

36. Anna M. Plonka, Tyler Grissom, Djamaladdin G. Musaev, Alex Balboa, Wesley O. Gordon, Daniel L. Collins Wildman, Sanjit K. Ghose, Yiyao Tian, Amani M. Ebrahim, Mark B. Mitchell, Craig L. Hill, John R. Morris, Anatoly I. Frenkel, “Effect of Carbon Dioxide on the Degradation of Chemical Warfare Agent Simulant in the Presence of Zr Metal Organic Framework MOF-808“, *Chem. Mater.,* **2019**, *31*, 9904-9914.

37. Brett D. McLarney, Steven R. Hanna, Djamaladdin G. Musaev, and Stefan France, “A Predictive Model for the $[Rh_2(esp)_2]$-catalyzed Intermolecular $C(sp^3)$-H bond insertion of β-carbonyl ester carbenes: Interplay Theory and Experiment“, *ACS Catalysis*, **2019**, 9, 4526-4538.

38. Alexey L. Kaledin, Craig L. Hill, Tianquan Lian, Djamaladdin G. Musaev, „Modulating Electronic Coupling at the Quantum Dot/Molecule Interface by Wavefunction Engineering“, *J. Chem. Phys.* **2019**, *150 (12),* 124704

39. Yiyao Tian, Anna M. Plonka, Amani M. Ebrahim, Robert M. Palomino, Sanjaya D. Senanayake, Alex Balboa, Wesley O. Gordon, Diego Troya, Djamaladdin G. Musaev, John R. Morris, Mark B. Mitchell, Daniel L. Collins-Wildman, Craig L. Hill, Anatoly I. Frenkel, „ A Correlated Multimodal Approach Reveals Key Details of Nerve-Agent Decomposition by Single Site Zr-Based Polyoxometalates.” *J. Phys. Chem. Lett*, **2019**, *10*, 2295-2299

40. Alexey L. Kaledin, Alex Balboa, Wesley O. Gordon, Diego Troya, John R. Morris, Mark B. Mitchell, Anatoly I. Frenkel, Craig L. Hill, Djamaladdin G. Musaev, „Key Mechanistic Details of Paraoxon Decomposition by Polyoxometalates: Critical Role of *Para*-Nitro Substitution”, *Chemical Physics*, **2019**, *518,* 30-37

41. Alexey L. Kaledin, MuthuKumar Kaliappan, Craig L. Hill, Djamaladdin G. Musaev “Effects of Surface Hydration on the Electron Injection Rate from Graphene to Anatase and Rutile TiO_2 Surfaces, *Chemical Physics*, **2019**, *526, 110463*

42. Joseph J. Gair, Brandon E. Haines, Alexander S. Filatov, Djamaladdin G. Musaev, Jared C. Lewis, „Di-Palladium Complexes are Active Catalysts for Mono-*N*-Protected Amino Acid Accelerated Enantioselective C-H Functionalization.”, *ACS Catalysis*, **2019**, 9, 11386-11397

2018

43. Jiantao Fu, Zhi Ren, John Bacsa, Djamaladdin G. Musaev, Huw M. L. Davies, „ Desymmetrization of Cyclohexanes by Site-Selective and Stereoselective C–H Functionalization“, *NATURE*, **2018**, *564 (7736), 395-397*

44. Brandon E. Haines, Richmond Sarpong, Djamaladdin G. Musaev, „On the Generality and Strength of Transition Metal β–effects“, *J. Am. Chem. Soc*., **2018**, *140,* 10612-10618.

45. Kuangbiao Liao, Yun-Fang Yang, Yingzi Li, Jacob N. Sanders, K. N. Houk, Djamaladdin G. Musaev, Huw M. L. Davies, „Design of catalysts for site-selective and enantioselective functionalization of non-activated primary C–H bonds“, *Nature Chem.*, **2018**, *10*, 1048-1055

46. Kenji Usui, Brandon E. Haines, Djamaladdin G. Musaev, Richmond Sarpong, „Understanding C–H functionalization site-selectivity in a directed alkynylation“, *ACS Catalysis*, **2018**, *8*, 4516-4527.

47. Brandon E. Haines, Brandon M. Nelson, Jessica Grandner, Justin Kim, Kendall N. Houk, Mohammad Movassaghi, Djamaladdin G. Musaev, „Mechanism of Permanganate Promoted

Dihydroxylation of Complex Diketopiperazines: Critical Roles of Counter-Cation and Ion-Pairing“, *J. Am. Chem. Soc*., **2018**, *140(41),* 13375-13386

48. Ajitha J. Manjaly, Fatima Pary, Toby L. Nelson, Djamaladdin G. Musaev, „Unveiling the role of base and additive in the Ullmann-type of arene-aryl C-C coupling reaction“, *ACS Catalysis*, **2018**, *8*, 4829-4837.

49. Brandon E. Haines, Jin-Quan Yu, Djamaladdin G. Musaev, “The Mechanism of Directed Ni(II)-Catalyzed C–H Iodination with Molecular Iodine”, *Chem. Sci.,* **2018**, *9*, 1144-1154

50. Wenbin Liu, Zhi Ren, Aaron T. Bosse, Kuangbiao Liao, Elizabeth L. Goldstein, John Bacsa, Djamaladdin G. Musaev, Brian M. Stoltz, Huw M. L. Davies, “Catalyst-Controlled Selective Functionalization of Unactivated C–H Bonds in the Presence of Electronically Activated C–H Bonds”, *J. Am. Chem. Soc.* **2018**, *140* (38), pp 12247–12255

51. Kuangbiao Liao, Wenbin Liu, Zachary L. Niemeyer, Zhi Ren, John Bacsa, Djamaladdin G. Musaev, Mathew S. Sigman, Huw M. L. Davies, “Site-Selective Carbene-Induced C–H Functionalization Catalyzed by Dirhodium Tetrakis(triarylcyclopropanecarboxylate) Complexes”, *ACS Catalysis*, **2018***, 8,* 678-682.

52. Alexey L. Kaledin, Darren M. Driscoll, Diego Troya, Daniel Collins-Wildman, Craig L. Hill, John R. Morris, Djamaladdin G. Musaev, “Impact of Ambient Gases on the Mechanism of the [$Cs_8Nb_6O_{19}$]-Catalyzed Nerve-Agent Decomposition”, *Chem. Sci.* **2018** ,*9*, 2147-2158

53. Sidney M. Wilkerson-Hill, Brandon E. Haines, Djamaladdin G. Musaev, and Huw M. L. Davies, „Synthesis of [3a,7a]-Dihydroindoles by a Tandem Arene Cyclopropanation/3,5-Sigmatropic Rearrangement Reaction**“** *J. Org. Chem*., **2018**, *83,* 7939-7949.

54. Daniel L. Collins-Wildman, Mooeung Kim, Kevin P. Sullivan, Djamaladdin G. Musaev, Craig L. Hill, „Buffer-induced acceleration and inhibition in polyoxometalate-catalyzed organophosphorus ester hydrolysis“, *ACS Catalysis*, **2018**, *8,* 7068-7076.

55. Alexey L. Kaledin, Dequi Kong, Kaifeng Wu, Tianquan Lian, Djamaladdin G. Musaev, „Quantum Confinement Theory of Auger-assisted Biexciton Recombination Dynamics in Type-I and quasi Type-II Quantum Dots“, *J. Phys. Chem. C*, **2018**, *122,* 18742 – 18750.

56. Kevin P. Sullivan, Qiushi Yin, Daniel L. Collins-Wildman, Meilin Tao, Yurii V. Geletii, Djamaladdin G. Musaev, Tianquan Lian, Craig L. Hill, „Multi-Tasking POM Systems“, *Fronties in Chemistry*, **2018**, *accepted*, doi: 10.3389/fchem.2018.00365

57. Zhi Ren, Travis L. Sunderland, Cecilia Tortoreto, Tzuhsiung Yang, John F. Berry, Djamaladdin G. Musaev, Huw M. L. Davies, „Comparison of Reactivity and Enantioselectivity between Chiral Bimetallic Catalysts: Bismuth-Rhodium and Dirhodium Catalyzed Carbene Chemistry“, *ACS Catalysis*, **2018**, *8(11)*, 10676-10682.

58. Justin A. Shapiro, Kelly R. Morrison, Shreya S. Chodisetty, Djamaladdin G. Musaev, William M. Wuest, „Biologically Inspired Total Synthesis of Ulbactin F, an Iron-Binding Natural Product“, *Org. Lett*, **2018**, *20 (18*), 5922-5926.

59. Adrián Varela-Álvarez, Brandon E. Haines and Djamaladdin G. Musaev, „Key Mechanistic Insights into the Intramolecular C-H Bond Amination and Double Bond Aziridination in Sulfamate Esters Catalyzed by Dirhodium Tetracarboxylate Complexes”, *J. of Organometallic Chem.,* **2018**, 867, 183-192

2017

60. Kuangbiao Liao, Tom Pickle, Vyacheslav Boyarskikh, John Bacsa, Djamaladdin G. Musaev, Huw M. L. Davies, „Site-selective and stereoselective functionalization of non-activated tertiary C–H bonds“, *NATURE*, **2017**, *551*, 609-613: DOI: 10.1038/nature24641

61. Joaquín Soriano-López, Djamaladdin G. Musaev, Craig Hill, José Ramón Galán-Mascarós, Jorge J. Carbó, Josep M. Poblet, „TetraCobalt-Polyoxometalate Catalysts for Water Oxidation: Key Mechanistic Details.“, *J. of Catalysis*, **2017**, *350*, 56-63.

62. Brandon E. Haines, Takahiro Kawakami, Kei Murakami, Kenichiro Itami, Djamaladdin G. Musaev, “Key Mechanistic Details and predictive Models for Cu-catalyzed Aromatic C-H Imidation with *N*-Fluorobenzenesulfonimide.” *Chem. Sci.,* 2017, 8 (2), 988-1002

63. Marika Wieliczko, Yurii V. Geletii, John Bacsa, Djamaladdin G. Musaev, Craig L. Hill, „Effects of Competitive Active-Site Ligand Binding on Proton- and Electron-Transfer Properties of the $[Co_4(H_2O)_2(PW_9O_{34})_2]^{10-}$ Polyoxometalate Water Oxidation Catalyst“, *J. Cluster Sci.*, 2017, 28 (2), 839-852

64. Brandon E. Haines, Jin-Quan Yu, Djamaladdin G. Musaev, „ An enantioselectivity model for Pd-catalyzed C-H Functionalization Mediated by the Mono-*N*-Protected Amino Acid (MPAA) Family of Ligands“, *ACS Catalysis*, 2017*, 7 (7)*, 4344-4354

65. Joseph J. Gair, Brandon E. Haines, Alexander S. Filatov, Djamaladdin G. Musaev, Jared C. Lewis, „ Remarkable dimeric structural motif of Palladium (II) mono-N-protected amino acid complexes and its importance in C-H Functionalization“, *Chem. Sci.,* 2017, *8 (8),* 5746-5756.

66. R. Erik Plata, David E. Hill, Brandon E. Haines, Djamaladdin G. Musaev, Ling Chu, David P. Hickey, Matthew S. Sigman, Jin-Quan Yu, Donna G. Blackmond “A Role for Pd(IV) in Catalytic Enantioselective C-H Functionalization With Monoprotected Amino Acid Ligands Under Mild Conditions” , *J. Am. Chem. Soc.* 2017, 139 (27), 9238-9245

67. Brett D. McLarney, Marchello A. Cavitt, Theodore M. Donnell, Djamaladdin G. Musaev, Stefan France, “Rh(II)-Catalyzed β-C(sp2)-H Alkylation of Enol Ethers, Enamides and Enecarbamates with α-Diazo Dicarbonyl Compounds”, *Chemistry-A European Journal*, 2017, 23 (5), 1129-1135

2016

68. Kuangbiao Liao, Solymar Negretti, Djamaladdin G. Musaev, John Bacsa, Huw M. L. Davies, “Site-selective and stereoselective Functionalization of unactivated C–H bonds,” *Nature,* **2016**, *533(7602)*, pp. 230-234.

69. Adrián Varela-Álvarez, Tzuhsiung Yang, Heather Jennings, Katherine P. Kornecki, Samantha N. MacMillan, Kyle M. Lancaster, James Booker Christianson Mack, Justin Du Bois, John F. Berry, Djamaladdin G. Musaev, “Rh_2(II,III) Catalysts with Chelating Carboxylate and Carboxamidate Supports: Electronic Structure and Nitrene Transfer Reactivity.” *J. Am. Chem. Soc.* **2016**, 138 (7), 2327-2341.

70. N. Mace Weldy, A. G. Schafer, C. P. Owens, C. J. Herting, A. Varela-Alvarez, S. Chen, Z. Niemeyer, D. G. Musaev, M. S. Sigman, H. M. L. Davies, S. B. Blakey, “ Iridium(III)-bis(imidazolinyl)phenyl catalysts for enantioselective C–H functionalization with ethyl diazoacetate.” *Chem. Sci.,* **2016,** *7 (5)*, pp. 3142-3146;

71. Yanyan Jia, Jinquan Chen, Kaifeng Wu, Alex Kaledin, Jamal Musaev, Zhaoxiong Xie, Tianquan Lian, “Enhancing Photo-reduction Quantum Efficiency Using Quasi-Type II Core/Shell Quantum Dots”, *Chem. Sci.,* **2016,** *7*, 4125-4133

72. Weiwei Guo, Hongjin Lv, Kevin P. Sullivan, Wesley O. Gordon, Alex Balboa, George W. Wagner, Djamaladdin G. Musaev, John Bacsa, Craig L. Hill, “Broad-Spectrum Liquid- and Gas-Phase

Decontamination of Chemical Warfare Agents by One-Dimensional Heteropolyniobates", *Angew. Chem. Int. Ed.,* **2016,** *55*, 7403-7407.

73. Elliot N. Glass, John Fielden, Zhuangqun Huang, Xu Xiang, Djamaladdin G. Musaev, Tianquan Lian, Craig L. Hill, " Transition Metal Substitution Effects on Metal-to-Polyoxometalate Charge Transfer." *Inorg. Chem.* **2016**, *55(9)*, pp. 4308-4319.

74. Robert C. Chapleski Jr., Djamaladdin G. Musaev, Craig L. Hill, and Diego Troya, "Reaction Mechanism of Nerve-Agent Hydrolysis with the $Cs_8Nb_6O_{19}$ Lindqvist Hexaniobate Catalyst." *J. Phys. Chem. C*, **2016,** *120 (30),* pp. 16822-16830

75. Brandon E. Haines, Yutaro Saito, Yasutomo Segawa, Kenichiro Itami, Djamaladdin G. Musaev, "Flexible Reaction Pocket on Bulky Diphosphine-Ir Complex Controls Regioselectivity in *para*-selective C-H Borylation of Arenes." *ACS Catalysis*, **2016**, *6 (11),* 7536-7546

76. Brandon E. Haines, John, F. Berry, Jin-Quan Yu, Djamaladdin G. Musaev, "Factors Controlling Stability and Reactivity of Dimeric Pd(II)-Complexes in C–H Functionalization Catalysis", *ACS Catalysis*, 2016, *6* (2), 829–839

77. Hongjin Lv, Yuanzhe Gao, Weiwei Guo, Sarah M Lauinger, Yingnan Chi, John Bacsa, Kevin P. Sullivan, Marika Wieliczko, Djamaladdin G Musaev, Craig L Hill, „Cu-based Polyoxometalate catalyst for efficient Catalytic Hydrogen Evalution", *Inorg. Chem.* 2016, *55*, pp. 6750-6758.

2015

78. Yurii Gueletii, J. Song, Hongjin Lv, Djamaladdin G Musaev, Zeng Luo, Craig L. Hill, „Photocatalytic Polyoxometalate compositions of tungstovanadates and uses as water oxidation catalysts", US Patent 20,150,298,100, **2015**

79. Djamaladdin G. Musaev, Brandon E. Haines „Factors Impacting the Mechanism of the Mono-N Protected Amino-Acid Ligand Assisted and Directing Group-Mediated CH Activation Catalyzed by Pd (II) Complex ", *ACS Catalysis.* **2015**, *5,* 830-840.

80. Kei Muto, Junichiro Yamaguchi, Djamaladdin G. Musaev, Kenichiro Itami, „Decarbonylative organoboron cross-coupling by nickel catalysis. The ester Suzuki–Miyaura coupling", *Nature Communication,* **2015**, *6*, 7508.

81. Alexey L. Kaledin, Tianquan Lian, Craig L. Hill, Djamaladdin G. Musaev, „A Hybrid Quantum Mechanical Approach: Intimate Details of Electron Transfer Between Type I CdSe/ZnS Quantum Dots and an Anthraquinone Molecule", *J. Phys. Chem. B,* **2015**, *119,* 7651-7658.

82. Brandon E. Haines, Huying Xu, Xiao-Chen Wang, Jin-Quan Yu, Djamaladdin G. Musaev, „Mechanistic Details of Pd(II)-Catalyzed C-H Iodination with Molecular I_2: Oxidative Addition vs Electrophilic Cleavage", *J. Am. Chem. Soc.* **2015**, *137*, 9022-9031.

83. John Fielden, Jordan M. Sumliner, Nannan Han, Yurii V. Geletii, Xu Xiang, Djamaladdin G. Musaev, Tianquan Lian, Craig L. Hill, „Water Splitting with Polyoxometalate-Treated Photoanodes: Enhancing Performance through Sensitizer Design", *Chem. Sci.,* **2015**, *6,* 5531-5543.

2014

84. Travis M. Figg, Sehoon Park, Juhyeon Park, Sukbok Chang, Djamaladdin G. Musaev, „Comparative Mechanistic Investigations of Direct C–H Amination of Benzamides Catalyzed by Cp*-Based Group 9 Metal Complexes", *Organometallics.* **2014**, *33* (15), pp 4076–4085.

85. Huiying Xu, Kei Muto, Junichiro Yamaguchi, Cunyuan Zhao, Kenichiro Itami, Djamaladdin G Musaev, „Key Mechanistic Features of Ni-catalyzed C–H/C–O Biaryl Coupling of Azoles and Naphthalen-2-yl Pivalates“, *J. Am. Chem. Soc.* **2014**, *136* (42), pp. 14834-14844.

86. Adrián Varela-Álvarez, Djamaladdin G. Musaev, "Fundamental Aspects of the Metal-Catalyzed C–H Bond Functionalization by Diazocarbenes: Guiding Principles for Design of Catalyst with Non-redox-Active Metal (Such as Ca) and Non-Innocent Ligand." In "*Understanding Organometallic Reaction Mechanisms and Catalysis. Experimental and Computational Tools*", Ed. Ananikov, V.; Wiley-VCH Verlag GmbH & Co. KGaA, **2014**, pp 17-40, Weinheim, Germany

87. Elliot N. Glass, John Fielden, Alexey L. Kaledin, Djamaladdin G. Musaev, Tianquan Lian, Craig L. Hill, „Extending Metal-to-Polyoxometalate Charge Transfer Lifetimes: The Effect of Heterometal Location*“ Chem.-A Eur. Journal*, **2014**, *20* (15), 4297-4307.

88. Hongjin Lv, Weiwei Guo, Kaifeng Wu, Zheyuan Chen, John Bacsa, Djamaladdin G Musaev, Yurii V Geletii, Sarah M Lauinger, Tianquan Lian, Craig L Hill, „A Noble-Metal-Free, Tetra-nickel Polyoxotungstate Catalyst for Efficient Photocatalytic Hydrogen Evolution", *J. Am. Chem. Soc.* **2014**, *136* (40), pp. 14015-14018.

89. Djamaladdin G. Musaev, Travis M. Figg, Alexey L. Kaledin, "Versatile Reactivity of Pd-Catalysts: Mechanistic Features of the Mono-N-Protected Amino-Acid Ligand and Cesium-Halide Base in Pd-Catalyzed C-H Bond Functionalization“ *Chem. Soc. Rev.* **2014**, *43,* 5009-5031. **DOI:** 10.1039/C3CS60447K

90. Hongjin Lv, Jie Song, Yurii V. Geletii, James W. Vickers, Jordan M. Sumliner, Djamaladdin G. Musaev, Paul Kögerler, Petro F. Zhuk, John Bacsa, Guibo Zhu, Craig L. Hill, „An Exceptionally Fast Homogeneous Carbon-Free Cobalt-Based Water Oxidation Catalyst“, *J. Am. Chem. Soc.* **2014**, *136* (26), pp. 9268-9271.

91. Alexey L. Kaledin, Tianquan Lian, Craig L. Hill, Djamaladdin G. Musaev, „An infinite order discrete variable representation of an effective mass Hamiltonian: Application to exciton wavefunctions in quantum confined nanostructures*.“ J. Theor. Comp. Chem.,* **2014**, 10 (8), pp 3409–3416.

92. Chongchao Zhao, Elliot N. Glass, Bryant Chica, Djamaladdin G. Musaev, Jordan M. Sumliner, R. Brian Dyer, Tianquan Lian, Craig L. Hill, "All-Inorganic Networks and Tetramer Based on Tin (II)-Containing Polyoxometalates: Tuning Structural and Spectral Properties with Lone-Pairs", *J. Am. Chem. Soc.* **2014**, 136 (34), 12085-12091.

2013

93. Chongchao Zhao, William Rodríguez-Córdoba, Alexey L. Kaledin, Ye Yang, Yurii V. Geletii, Tianquan Lian, Djamaladdin G. Musaev, Craig L. Hill, "An Inorganic Chromophore Based on a Molecular Oxide Supported Metal Carbonyl Cluster: $[P_2W_{17}O_{61}\{Re(CO)_3\}_3\{ORb(H_2O)\}(\mu_3\text{-}OH)]^{9-}$ ",*Inorg. Chem.* **2013**, *52* (23), pp 13490–13495

94. Hongjin Lv, Jennifer A. Rudd, Petro F. Zhuk, Ji Young Lee, Edwin C. Constable, Catherine E. Housecroft, Craig L. Hill, Djamaladdin G. Musaev, Yurii V. Geletii „Bis(4 '-(4-pyridyl)-2,2 ':6 ',2 "-terpyridine) ruthenium(II) complexes and their N-alkylated derivatives in catalytic light-driven water oxidation“ *RSC ADVANCES*, **2013**, *3* (43), pp. 20647-20654

95. James W. Vickers, Hongjin Lv, Jordan M. Sumliner, John Fielden, Guibo Zhu, Zhen Luo, Djamaladdin G. Musaev, Yurii V. Geletii, Craig L. Hill, „ Hydrolytic stability studies of $[Co_4(H_2O)_2(\alpha\text{-}PW_9O_{34})_2]^{10-}$. Additional evidence that transition-metal substituted polyoxometalates are molecular water oxidation catalysts.“, *J. Am. Chem. Soc*., 2013, *135* (38), pp. 14110–14118

96. Hongjin Lv, Jie Song, Haiming Zhu, Yurii V. Geletii, John Bacsa, Chongchao Zhao, Tianquan Lian, Djamaladdin G. Musaev, and Craig L. Hill „Visible-Light-Driven Hydrogen Evolution from Water Using a Noble-Metal-Free Polyoxometalate Catalyst“, *J. of Catalysis,* **2013**, *307, 48-54*

97. Travis M. Figg, Masayuki Wasa, Jin-Quan Yu, Djamaladdin G. Musaev, „Understanding the reactivity of Pd(0)/PR_3 catalyzed intermolecular C(sp^3)-H bond arylation,“ *J. Am. Chem. Soc.* **2013**, *135* (38), pp. 14206–14214

98. Chongchao Zhao, Choon Sung Kambara, Ye Yang, Alexey L. Kaledin, Djamaladdin G. Musaev, Tianquan Lian, and Craig L. Hill, „Synthesis, Structures, and Photochemistry of Tricarbonyl Metal Polyoxoanion Complexes, $[X_2W_{20}O_{70}\{M(CO)_3\}_2]^{12-}$ (X = Sb, Bi and M = Re, Mn)“, *Inorg. Chem.*, **2013**, *52* (2), pp 671–678

99. Adrián Varela-Álvarez, Djamaladdin G. Musaev, “Can the bis(imino)pyridine Iron, (PDI)FeL^1L^2, Complex Catalyze C-H Bond Functionalization?”, *Chem Sci.,* **2013**, *4*(9), 3758-3764

100. Hengbin Wang, David M. Guptill, Adrian Varela Alvarez, Djamaladdin G. Musaev, Huw M. L. Davies, “Rhodium-catalyzed enantioselective cyclopropanation of electron deficient alkenes”, *Chem Sci.,* 2013, *4(7)*, pp 2844-2850

101. Xu Xiang, John Fielden, William Rodríguez-Córdoba, Zhuangqun Huang, Naifei Zhang, Zhen Luo, Djamaladdin G. Musaev, Tianquan Lian, and Craig L. Hill, „Electron Transfer Dynamics in Semiconductor–Chromophore–Polyoxometalate Catalyst Photoanodes“ *J. Phys. Chem. C*, **2013**, *117* (2), pp 918–926

102. Clayton P. Owens, Adrián Varela-Álvarez, Vyacheslav Boyarskikh, Djamaladdin G. Musaev, Huw M. L. Davies, Simon B. Blakey, “Iridium(III)-bis(oxazolinyl)phenyl Catalysts for Enantioselective C-H Functionalization“, *Chem Sci.,* **2013**, *4(6)*, pp 2590-2596

103. Benjamin Matt, Xu Xiang, Alexey L. Kaledin, Nannan Han, Jamal Moussa, Hani Amouri, Sandra Alves, Craig L. Hill, Tianquan Lian, Djamaladdin G. Musaev, Guillaume Izzet and Anna Proust, „Long lived charge separation in iridium(III)-photosensitized polyoxometalates: synthesis, photophysical and computational studies of organometallic–redox tunable oxide assemblies“, *Chem. Sci.*, **2013**, *4(4)*, pp 1737-1745

104. Alexey L. Kaledin, Adri C. T. van Duin, Craig L. Hill, Djamaladdin G. Musaev „Parameterization of Reactive Force Field: Dynamics of the $[H_xNb_6O_{19}]^{(8-x)}$ Lindqvist Polyoxoanion in Bulk Water“, *J. Phys. Chem. A*, **2013**, *117, 32,* 6967-6974

2012

105. Alexey L. Kaledin, Tianquan Lian, Craig L. Hill, and Djamaladdin G. Musaev, „Structural Modification of TiO_2 Surfaces in Bulk Water and Binding Motifs of a Functionalized C_{60} on TiO_2 Anatase and Rutile Surfaces in Vacuo and in Water: Molecular Dynamics Studies“, *J. Phys. Chem. C*, **2012**, *116* (39), pp 20937–20948

106. Lv, Hongjin; Geletii, Yurii V.; Zhao, Chongchao: Vickers, James W.; Zhu, Guibo; Luo, Zhen;Song, Jie; Lian, Tianquan; Musaev, Djamaladdin G.; Hill, Craig L. „Polyoxometalate water oxidation catalysts and the production of green fuel,“ *Chem. Soc. Rev.*, **2012**, *41*, Issue: 22, 7572-7589

107. Adrián Varela-Álvarez, Lanny S. Liebeskind, and Djamaladdin G. Musaev, „Mechanistic Insights into the Aerobic Copper(I)-Catalyzed Cross-Coupling of *S*-Acyl Thiosalicylamide Thiol Esters and Boronic Acids“, *Organometallics*, **2012**, *31* (22), pp 7958–7968

108. Zhanjie Li, Vyacheslav Boyarskikh, Jørn H. Hansen, Jochen Autschbach, Djamaladdin G. Musaev, and Huw M. L. Davies, „Scope and Mechanistic Analysis of the Enantioselective Synthesis of

Allenes by Rhodium-Catalyzed Tandem Ylide Formation/[2,3]-Sigmatropic Rearrangement between Donor/Acceptor Carbenoids and Propargylic Alcohols“, *J. Am. Chem. Soc,* **2012**, *134,* 15497-15504

109. Zhuangqun Huang, Yongjing Lin, Xu Xiang, William Rodríguez-Córdoba, Kenneth J. McDonald, Karl S. Hagen, Kyoung-Shin Choi, Bruce S. Brunschwig, Djamaladdin G. Musaev, Craig L. Hill, Dunwei Wang, and Tianquan Lian *“In situ* probe of photocarrier dynamics in water-splitting hematite (alpha-Fe2O3) electrodes“, *Energy & Environmental Science*, **2012**, *v.5, issue 10, 8923-8926*

110. Djamaladdin G. Musaev, Alexey Kaledin, Bing-Feng Shi, Jin-Quan Yu, „ On the origin of enantioselectivity of the Pd(II)-catalyzed C-H bond activation reactions: A combined experimental and computational approach“ , *J. Am. Chem. Soc,* **2012**, *134,* 1690-1698

111. Djamaladdin G. Musaev, Simon B. Blakey, „A DFT computational study reveals key mechanistic feartures of Ruthenium-pybox catalyzed C-H amination“ *Organometallics,* **2012**, *31,* 4950-4961

112. Valentine P. Ananikov, Nikolay V. Orlov, Sergey S. Zalesskiy, Irina P. Beletskaya, Victor N. Khrustalev, Keiji Morokuma and Djamaladdin G. Musaev, „ Catalytic Adaptive Recognition of Thiol (SH) and Selenol (SeH) Groups Towards Synthesis of Functionalized Vinyl Monomers“,*J. Am. Chem. Soc,* **2012**, *134,* 6637-6649 *(see also: Chemical & Eng. News, 2012, April 16, page 40)*

113. Zhuangqun Huang, Yurii V. Geletii, Djamaladdin G. Musaev, Craig L. Hill, and Tianquan Lian, “Spectroscopic Studies of Light-driven Water Oxidation Catalyzed by Polyoxometalates“, *Industrial & Engineering Chemistry Research*, **2012**, *v. 51, issue 37*, 11850-11859

114. Guibo Zhu, Elliot N. Glass, Chongchao Zhao, Hongjin Lv, James W. Vickers, Yurii V. Geletii, Djamaladdin G. Musaev, Craig L. Hill „ A soluble and stable Ni-based water oxidation catalyst for solar fuel production“, *Dalton Trans*, **2012**, *41*, 13043 - 13049.

115. Guibo Zhu, Elliot N. Glass, Chongchao Zhao, Yurii V. Geletii, Djamaladdin G. Musaev, Craig L. Hill, „A Novel Dodecanuclear Zn^{II} Cluster Sandwiched by Polyoxometalate Ligands“,*Dalton Trans*, **2012** , *41*, 9908-9913.

116. Zhu, Guibo; Geletii, Yurii V.; Koegerler, Paul; Schilder, Helmut; Song, Jie; Lense, Sheri; Zhao, Chongchao; Hardcastle, Kenneth I.; Musaev, Djamaladdin G.; Hill, Craig L. „ Water oxidation catalyzed by a new tetracobalt-substituted polyoxometalate complex: $[\{Co_4(mu\text{-}OH)(H_2O)_3\}(Si_2W_{19}O_{70})]^{11-}$“ *Dalton Trans*, **2012**, *41*, 2084-2090.

117. Kevin P. O’Halloran, Chongchao Zhao, Nicole S. Ando, Arthur J. Schultz, Thomas F. Koetzle, Paula M. B. Piccoli, Britt Hedman, Keith O. Hodgson, Elena Bobyr, Martin L. Kirk, Sushilla Knottenbelt, Ezra C. Depperman, Benjamin Stein, Travis M. Anderson, Rui Cao, Yurii V. Geletii, Kenneth I. Hardcastle, Djamaladdin G. Musaev, Wade A. Neiwert, Xikui Fang, Keiji Morokuma, Shaoxiong Wu, Paul Kögerler, and Craig L. Hill „ Revisiting the Polyoxometalate-Based Late-Transition-Metal-Oxo Complexes: The “Oxo Wall” Stands“, *Inorg. Chem.*, **2012**, *51,* 7025-7031

2011

118. Mark Edwin Harvey, Djamaladdin G. Musaev, J. Du Bois „A diruthenium catalyst for selective allulyc C-H amination: Reaction development and mechanistic insight gained through experiment and theory“ *J. Am. Chem. Soc,* **2011**, *133,* 17207-17216

119. Chongchao Zhao, Zhuangqun Huang, William Rodríguez-Córdoba, Choon Sung Kambara, Kevin P. O’Halloran, Ken I. Hardcastle, Djamaladdin G. Musaev, Tianquan Lian, and Craig L. Hill

„Synthesis and characterization of a Metal-to-Polyoxometalate charge transfer molecular chromophore“, *J. Am. Chem. Soc,* **2011**, *133,* 20134-20137

120. Changming Qin, Vyacheslav Boyarskikh, Jørn H. Hansen, Kenneth E. Hardcastle, Djamaladdin G. Musaev, Huw M. L. Davies, “D2-symmetric dirhodium catalyst derived from a 1,2,2-triarylcyclopropane carboxylate ligand: Design, synthesis and application”, *J. Am. Chem. Soc,* **2011**, *133,* 19198-19204

121. A E. Kuznetsov, Y. V. Geletii, C. L. Hill, K. Morokuma, D. G. Musaev, „The Effect of the Heteroatom on the Reactivity of Di-Ru-substituted Polyoxometalates $\{\gamma\text{-}[Ru^{III}(\mu\text{-}OH)_2Ru^{III}][(X^{n+}O_4)W_{10}O_{32}]\}^{(8-n)-}$ Towards Dioxygen and Water Activation: Comparison of X = P^V and S^{VI} with Si^{IV}“, *Theo. Chem Acc.,* **2011**, 130, 197-207.

122. Guibo Zhu, Yurii V. Geletii, Paul Kögerler, Helmut Schilder, Jie Song, Sheri Lense, Chongchao Zhao, Kenneth I. Hardcastle, Djamaladdin G. Musaev, Craig L. Hill, “Water oxidation catalyzed by a new tetracobalt-substituted polyoxometalate complex: $[\{Co_4(\mu\text{-}OH)(H_2O)_3\}(Si_2W_{19}O_{70})]^{11-}$ “, *Dalton Trans.,* **2011**, *41,* 2084-2090.

123. Wenchao Zhang, Yanhui Tang, Ming Lei, Keiji Morokuma, Djamaladdin G. Musaev, „Ditantalum dinitrogen complex: Reaction of H_2 molecule with „end-on-bridged“ $[Ta^{IV}]_2(\mu\text{-}\eta^1\text{:}\ \eta^1\text{-}N_2)$ and bis(-nitrido) $[Ta^{IV}]_2(\mu\text{-}N)_2$ and complexes.“ *Inorg. Chem.* **2011**, *50*, 9481-9490.

124. Zhuangqun Huang, Zhen Luo, Yurii V. Geletii, James Vickers, Qiushi Yin, David Wu, Yu Hou, Yong Ding, Djamaladdin G. Musaev, Craig L. Hill, Tianquan Lian, „Efficient light-driven carbon-free Cobalt-based molecular catalyst for water oxidation“ *J. Am. Chem. Soc,* **2011**, *133,* 2068-2071.

125. Yurii V. Geletii, Qiushi Yin, Yu Hou, Zhuangqun Huang, Huiyuan Ma, Jie Song, Claire Besson, Zhen Luo, Rui Cao, Kevin P. O_Halloran, Guibo Zhu, Chongchao Zhao, James W. Vickers, Yong Ding, Sajjad Mohebbi, Aleksey E. Kuznetsov, Djamaladdin G. Musaev, Tianquan Lian, Craig L. Hill, “Polyoxometalates in the design of effective and tunable water oxidation catalyst”, *Isr. J. Chem.,* **2011**, *51*, pp 238-246

2010

126. Krishna K. Pandey, Djamaladdin G. Musaev, “Structure and Bonding Energy Analysis of Cobalt, Rhodium and Iridium Borylene Complexes $[(\eta^5\text{-}C_5H_5)(CO)M(BNX_2]$, (X = Me, SiH_3, $SiMe_3$) and $[(\eta^5\text{-}C_5H_5)(PMe_3)M\{BN(SiH_3)_2\}]$ (M = Co, Rh, Ir) “, *Organometallics* **2010**, *29* (1), pp 142–148

127. Jie Song, Zhen Luo, Haiming Zhu, Zhuangqun Huang, Tianquan Lian, Alexey L. Kaledin Djamaladdin G. Musaev, Sheri Lense, Kenneth Hardcastle, Craig L. Hill „Synthesis, structure and characterization of two polyoxometalate-photosensitizer hybrid materials“, *Inorg. Chem. Acta*, **2010**, *363,* pp 4381 – 4386

128. A. E. Kuznetsov, D. G. Musaev, „Does the MgO(100)-support facilitate the reaction of dinitrogen and dihydrogen molecules catalyzed by Zr_2Pd_2 Clusters? A Computational Study“, *Inorg. Chem.*, **2010**, *49,* pp 2557-2567

129. David Quinonero, Alexey Kaledin, Aleksey E. Kuznetsov, Yurii, V. Geletii, Claire Besson, Craig L. Hill, Djamaladdin G. Musaev, „Computational studies of the geometry and electronic structure of an all-inorganic and homogeneous tetra-Ru-polyoxometalate catalyst for water oxidation and ist four subsequent one-electron oxidized forms“, *J. Phys. Chem. A.,* **2010**, *114* (1), pp 535–542

130. Alexey L. Kaledin, Tianquan Lian, Yurii V. Geletii, Craig L. Hill, and Djamaladdin G. Musaev, „ Insights into photoinduced electron transfer between $[Ru(bpy)_3]^{2+}$ and $S_2O_8^{2-}$ in water: computational and experimental studies “, *J. Phys. Chem. A.,* **2010**, *114* (1), pp 73-80.

131. Valentine P. Ananikov, Djamaladdin G. Musaev, Keiji Morokuma, "Real size of ligands, substrates and catalysts: studies of structure, reactivity and selectivity by ONIOM and other hybrid computational approaches", *J. Mol. Catalysis A,* **2010**, *324(1-2),* pp 104-119

132. C. Besson, Z. Huang, Y. V. Geletii, S. Lense, K. I. Hardcastle, D. G. Musaev, T. Lian, A. Proust, C. L. Hill, "$Cs_9[(\gamma\text{-}PW_{10}O_{36})_2Ru_4O_5(OH)(H_2O)_4]$, a new all-inorganic, soluble catalyst for the efficient visible-light-driven oxidation of water " *Chem. Comm.* **2010**, 46, 2784-2786.

133. Alexey L. Kaledin, Zhuangqun Huang, Qiushi Yin, Emma L. Dunphy, Edwin C. Constable, Catherine E. Housecroft, Yurii V. Geletii, Tianquan Lian, Craig L. Hill, Djamaladdin G. Musaev „Insights into Photoinduced Electron Transfer Between $[Ru(mptpy)_2]^{4+}$ (mptpy = 4'(4-methylpyridinio)-2,2':6',2"-terpyridine) and $[S_2O_8]^{2-}$: Computational and Experimental Studies", *J. Phys. Chem. A,* **2010**, *114,* pp 6284-6297.

134. Aleksey E. Kuznetsov, Yurii V. Geletii, Craig L. Hill, Djamaladdin G. Musaev, „Insights into mechanism of O2 formation and release from the $Mn_4O_4L_6$ „cubane" cluster". *J. Phys. Chem. A,* **2010**, *114,* pp 11417 – 11424.

135. Qiushi Yin, Jeffrey Miles Tan, Claire Besson, Yurii V. Geletii, Djamaladdin G. Musaev, Aleksey E. Kuznetsov, Zhen Luo, Ken I. Hardcastle, Craig L. Hill „A soluble molecular fast organic-structure-free water oxidation catalyst based on abundant metals" *Science,* **2010**, *328,* 342-345

136. Krishna K. Pandey, James P. Snyder, Dennis C. Liotta, Djamaladdin G. Musaev, "Transition Metal Selectivity of Octapeptide Repeat Region of Prion Protein (PrP): The Computation Studies", *J. Phys. Chem.* B, **2010,** 114, 1127-1135

2009

137. A. E. Kuznetsov, Y. V. Geletii, C. L. Hill, K. Morokuma, D. G. Musaev, „Mechanism of the Divanadium-Substituted Polyoxotungstate $[\gamma\text{-}1,2\text{-}H_2SiV_2W_{10}O_{40}]^{4-}$ Catalyzed Olefin Epoxidation by H_2O_2: A Computational Study", *Inorg. Chem.* **2009**, *48,* 1871-1878

138. Kuznetsov, A. E.; Geletii, Y. V.; Hill, C. L.; Morokuma, K.; Musaev, D. G. " Dioxygen and Water Activation Processes on Multi-Ru-substituted Polyoxometalates: Comparison with the "Blue Dimer" Water Oxidation Catalyst" *J. Am. Chem. Soc.* **2009**, *131,6844-6854.*

139. Y. V. Geletii, C. Besson, Y. Hou, Q. Yin, D. G. Musaev, D. Quinonero, R. Cao, K. I. Hardcastle, A. Proust, P. Kogerler, C. L. Hill, „ Structural, Physicochemical and Reactivity Properties of and All-Inorganic Catalyst for Water Oxidation", *J. Am. Chem. Soc.* **2009**, *131,* 17360-17370.

140. S. C. Xu, S. Irle, D. G. Musaev, M. C. Lin, "Quantum Chemical Prediction of Pathways and Rate Constants for Reactions of CO and CO_2 with Vacancy Defects on Graphite (0001) Surfaces", *J. Phys. Chem.* C, **2009**, *113* (43), pp 18772–18777.

141. Claire Besson, Djamaladdin G. Musaev, Vanina Lahootun, Rui Cao, Lise-Marie Chamoreau, Richard Villanneau, Françoise Villain, René Thouvenot, Yurii V. Geletii, Craig L. Hill, Anna Proust, "Vicinal di-nitridoruthenium substituted polyoxometalates, g-$[XW_{10}O_{38}\{RuN\}_2]^{6-}$ (X=Si or Ge)" *Eur. J. Chem.* **2009**, *15*, 10233-10243.

142. Djamaladdin G. Musaev, Lanny S. Liebeskind, „On the Mechanism of Pd(0)-Catalyzed, Cu(I) Carboxylate-Mediated Thioorganic-Boronic Acid Coupling. A Noninnocent Role for Carboxylate Ligand",*Organometallics,* **2009,** *28, 4639-4642*

143. David Quinonero, Djamaladdin G. Musaev, Keiji Morokuma, „Computational insights to the mechanism of alkene epoxidation by mangenes-based catalysts in the presence of bicarbonate", *J. Molecular Structure: THEOCHEM*, **2009**, *903(1-3),* 115-122

144. Gabriella Tamasi, Renzo Cini, Djamaladdin G. Musaev, Keiji Morokuma, „ An Experimental and Density Functional Study of the Sb-C Bond Activation and Organo-Rh Bond Formation from the Spontaneous Decay of $[RhCl_3(SbPh_3)_3]$", *Polyhedron*, **2009**, *28,* 3675-3684.

145. Yukiko Sakimoto, Kimihiko Hirao, Djamaladdin G. Musaev, „Theoretical insights inot the thiol reductase activity of Ebtellur.", *Int. J. Quantum Chemistry*, **2009**, *109 (10),* 2297-2307.

146. Hsin-Tsung Chen, Hui-Lung Chen, Shin-Pon Ju, Djamaladdin G. Musaev, M. C. Lin, „ Density–Functional Studies of the Adsorption and Dissociation of NO_x (x=1, 2) molecules on W(111) Surface", *J. Phys. Chem. C.* **2009**, *113,* 5300-5307

147. Yurii V. Geletii, Zhuangqun Huang, Yu Hou, Djamaladdin G. Musaev, Tianquan Lian, Craig L. Hill, „Homogeneous Light-Driven Water Oxidation Catalyzed by an Organic-Structure-Free Tetraruthenium Complex", *J. Am. Chem. Soc.,* **2009**, *131,* 7522-7523

2008

148. Traves M. Anderson, Rui Cao, Elena Slonkina, Britt Hedman, Keith O. Hodgson, Kenneth I. Hardcastle, Wade A. Neiwert, Shaoxiong Wu, Martin L. Kirk, Sushilla Knottenbelt, Ezra C. Depperman, Bineta Keita, Louis Nadjo, Djamaladdin G. Musaev, Keiji Morokuma, Craig L. Hill, „A Palladium-oxo complex. Stabilization of this proposed catalytic intermediate by an encapsulating polytungstate ligand", *J. Amer. Chem. Soc,* **2008**, *130,* 2877-2879

149. Yurii V. Geletii, Bogdan Botar, Paul Kogerler, Daniel A. Hillesheim, Djamaladdin G. Musaev, Craig L. Hill, „An All-Inorganic, Stable, and Highly Active Tetraruthenium Homogenous Catalyst for Water Oxidation", *Angew. Chem. Intern. Ed.* **2008**, *47,* 3896-3899

150. Jerzy Moc, Djamaladdin G. Musaev, Keiji Morokuma, "Zeolite-Supported Palladium Tetramer and Its Reactivity toward H2 Molecules: Computational Studies" *J. Phys. Chem. A.* **2008**, *112,* 5973-5983

151. Hui-Lung Chen, Shin-Pon Ju, Hsin-Tsung Chen, Djamaladdin G. Musaev, M. C. Lin, "Adsorption and Dissociation of the HCl and Cl2 Molecules on W(111) Surface: A Computational Study", *J. Phys. Chem. C.* **2008**, *112,* 12342-12348

152. Hsin-Tsung Chen, Djamaladdin G. Musaev, M. C. Lin, „Adsorption and Dissociation of CO_x (x=1, 2) on W(111) surface: A Computational Study", *J. Phys. Chem. C.* **2008**, *112,* 3341-3349.

153. Hsin-Tsung Chen, Jee-Gong, Chang, Djamaladdin G. Musaev, M. C. Lin, "A Computational Study on kinetics and mechanisms of unimolecular decomposition of succinic acid and its anhydride", *J. Phys. Chem. A.* **2008**, *112,* 6621-6629

154. Prabhakar, R.; Morokuma. K.; Musaev. D. G. „Computational Insights into the Structural Properties and Catalytic Functions of Selenoprotein Glutathione Peroxidase (GPx)." In *Computational Modeling for Homogenous and Enzymatic Catalysis,* Eds: Morokuma, K. and Musaev, D. G.; Weinheim, Germany; Wiley-VCH., **2008**, 1-25

155. Musaev, D. G.; Bobadova-Parvanova, P.; Morokuma, K. „The Principles of Dinitrogen Hydrogenation: Computational Insights." In *Computational Modeling for Homogenous and Enzymatic Catalysis,* Eds: Morokuma, K. and Musaev, D. G.; Weinheim, Germany; Wiley-VCH., **2008**, 83-108

156. Valentine P. Ananikov, Djamaladdin G. Musaev and Keiji Morokuma, „Transition metal catalyzed carbon-carbon bond formation: the key of homogeneous catalysis", In *Computational Modeling for Homogenous and Enzymatic Catalysis,* Eds: Morokuma, K. and Musaev, D. G.; Weinheim, Germany; Wiley-VCH., **2008**, 131-148

157. Rajeev Prabhakar, Keiji Morokuma, Yurii V Geletii, Craig L. Hill, and Djamaladdin G. Musaev, "Insights into the Mechanism of H_2O_2-based Olefin Epoxidation Catalyzed by the Lacunary [γ-$(SiO_4)W_{10}O_{32}H_4]^{4-}$ and di-V-substituted-γ-Keggin [γ-1,2-$H_2SiV_2W_{10}O_{40}]^{4-}$ Polyoxometalates. A Computational Study." In *Computational Modeling for Homogenous and Enzymatic Catalysis,* Eds: Morokuma, K. and Musaev, D. G.; Weinheim, Germany; Wiley-VCH., **2008**, 215-230

158. Rui Cao, Jong Woo Han, Traves M. Anderson, Daniel A. Hillesheim, Martin L. Kirk, Djamaladdin G. Musaev, Keijji Morokuma, Yurii V. Geletii, Craig L. Hill, „ Late Transition Metal Oxo Compounds and Open Framework Materials that Catalyze Aerobic Oxidations", *Prog. Inorg. Chem.,* **2008**, *60,* 245-272.

2007

159. Sonia Martinez, Keiji Morokuma, and Djamaladdin G. Musaev „Mechanistic Aspects of Dinitrogen Hydrogenation Catalyzed by the Geometry Constrained-Zirconium and Titanium Complexes: Computational Studies."*Organometallics,* **2007**, *26,* 5978-5986.

160. Valentine P. Ananikov, Djamaladdin G. Musaev and Keiji Morokuma "Critical Effects of Phosphine Ligands on the Mechanism of Carbon-Carbon Bond Formation Involving Palladium(II) Complexes. A Theoretical Evaluation of Steric and Electronic Factors" *Eur. J. Inorg. Chem* **2007**, *34,* 5390-5399

161. Lei Shi, Dan E. Lundberg, Djamaladdin G. Musaev, and Fredric M. Menger, "[12]Annulene Geminis: Computations, NMR Diffusometry, and Self-Asssembly", *Angew. Chem. Intern. Ed.* **2007**, *46,* 5889-5891.

162. Xu, S. C.; Irle, S.; Musaev, D. G.; Lin, M. C. „ Quantum Chemical Study of the Dissociative Adsorption of OH and H_2O on Pristine and Defective Graphite (0001) Surfaces: Reaction Mechanism and Kinetics"*J. Phys. Chem. B.* **2007**, *111,* 1355-1365.

163. Hsin-Tsung Chen, Djamaladdin G. Musaev, Stephan Irle and M. C. Lin, "Mechanisms of the Reactions of W and W+ with NOx (x = 1, 2): A Computational Study" *J. Phys. Chem. A.,* **2007**, *111*, 982-991.

164. D. G. Musaev, Stephan Irle, and M. C. Lin, "The Mechanisms of the Reactions of W and W^+ with CO_x (x = 1, 2): A Computational Study", *J. Phys. Chem. A,* **2007**, 111(29); 6665-6673.

165. Hsin-Tsung Chen, Djamaladdin G. Musaev, and M. C. Lin, „Adsorption and Dissociation of H_2O on W(111) surface: A Computational Study" *J. Phys. Chem. c.*, **2007,** *111,* 17333-17339.

166. Hill, C. L.; Delannoy, L.; Duncan, D. C.; Weinstock, I. A.; Renneke, R. F.; Reiner, R. S.; Atalla, R. H.; Han, J. W.; Hillesheim, D. A.; Cao, R.; Anderson, T.; Okun, N. M.; Musaev, D. G.; Geletii, Y. "Complex catalysts from self repairing ensembles to highly reactive air-based oxidation systems" *Comptes Rendus Chimie*, **2007**, *10*, 305-312

167. Quiñonero, D.; Morokuma, K.; Geletii, Y. V.; Hill, C. L.; Musaev, D. G. "A Density Functional Study of Geometry and Electronic Structure of $[(SiO_4)(M^{III})_2(OH)_2W_{10}O_{32}]^{4-}$ for M = Mo, Ru and Rh." *J. Mol. Catal. A, Chem*. **2007**, 262, 227-235.

168. Nowroozi-Isfahani, R.; Musaev, D. G.; Morokuma, K.; Gagne, M. R. „ Density Functional Study of Platinum(II)-Mediated Bicyclization of 1,6-Dienylphenols", *Organometallics*, **2007**, *26*, 2540-2549

169. Cao, R.; Anderson, T. M.; Piccoli, P. M. B.; Schultz, A. J.; Koetzle, T. F.; Geletii, Y. V.; Slonkina, E.; Hedman, B.; Hodgson, K. O.; Hardcastle, K. I.; Fang, X.; Kirk, M. L.; Knottenbelt, S.; Kögerler, P.; Musaev, D. G.; Morokuma, K.; HilL, C. L. „Reactive terminal gold-oxo units"*J. Am. Chem. Soc.*, **2007**, 129(36); 11118-11133..

170. Zheng, G.; Witek, H.; Bobadova-Parvanova, P.; Irle, S.; Musaev, D. G.; Prabhakar, R.; Morokuma, K.; Lundberg, M.; Elstner, M.; Köhler, C.; Frauenheim, T. „Parameterization of Transition Metal Elements for the Spin-Polarized Self-Consistent-Charge Density-Functional Tight-Binding Method: 1. Parameterization of Ti, Fe, Co, and Ni.“ *J. Chem. Theory and Comp.,* **2007**, 3(4); 1349-1367.

171. Khoroshun, D. V.; Musaev, D. G.; Morokuma, K. ”Electronic reorganization: origin of sigma trans promotion effect” *J. Comput. Chem*. **2007**, *28,* 423-441.

172. Musaev, D. G.; Bobadova-Parvanova, P.; Morokuma, K. „Why $[(\eta^5\text{-}C_5Me_nH_{5\text{-}n})_2Ti]_2(\mu_2, \eta^2, \eta^2\text{-}N_2)$ Can Not Add a H_2 Molecule to the Side-On-Coordinated N_2 while Its Zr and Hf Analogues Can? Insights from Computational Studies“ *Inorg. Chem.;* **2007**; *46,* 2709-2715.

2006

173. Prabhakar, R.; Morokuma, K.; Hill, C. L**.; Musaev, D. G.** ”Insights into the Mechanism of Selective Olefin Epoxidation Catalyzed by $[\gamma\text{-}(SiO_4)W_{10}O_{32}H_4]^{4-}$. A Computational Study” *Inorg. Chem.* **2006**, 45 (14), 5703 – 5709.

174. Xu, S. C.; Irle, S.; Musaev, D. G.; Lin, M. C. „Quantum Chemical Prediction of Reaction Pathways and Rate Constants for Dissociative Adsorption of COx and NOx on the Graphite (0001) Surface“ *J. Phys. Chem. B.* **2006**; 110, 21135-21144.

175. Nowroozi-Isfahani, T.; Musaev, D. G.; Morokuma, K.; Rosenberg, E. „Computational Studies of Nucleophilic Attack and Protonation of Electron-Deficient Benzoheterocycle Triosmium Clusters“ *Inorg. Chem.* **2006**, 45 (13); 4963-4973.

176. Botar, B.; Geletii, Y. V.; Kogerler, P.; Musaev, D. G.; Morokuma, K.; Weinstock, I. A.; Hill, C. L. ” The True Nature of the Diiron(iii) γ-Keggin Structure in Water. Catalytic Aerobic Oxidation and Chemistry of an Unsymmetric Trimer” *J. Am. Chem. Soc.* **2006**, 128 (34), 11268-11277.

177. Hill, C. L.; Anderson, T. M.; Han, J. W.; Hillesheim, D. A.; Geletii, Y. V.; Okun, N. M.; Cao, R.; Botar, B.; Musaev, D. G.; Morokuma, K. “New complexes and materials for O_2-based oxidations” *J. Mol. Catal. A. Chem.* **2006**, 251(1-2), 234-238.

178. Prabhakar, R.; Morokuma, K.; Musaev, D. G. ” Peroxynitrite Reductase Activity of Selenoprotein Glutathione Peroxidase: A Computational Study”, *Biochemistry,* **2006**, 45 (22), 6967-6977.

179. Prabhakar, R.; Vreven, T.; Frisch, M. J.; Morokuma, K.; Musaev, D. G. ” Is the Protein Surrounding the Active-Site Critical for Hydrogen Peroxide Reduction by Selenoprotein Gkutathione Peroxidase (GPx)? An ONIOM Study”, *J. Phys. Chem. B*, **2006**, 110 (27), 13608-13613.

180. Bobadova-Parvanova, P.; Wang, Q.-F.; Quinonero-Santiago, D.; Morokuma, K.; Musaev, D. G. „Does Dinitrogen Hydrogenation Follow Different Mechanism for $[(\eta^5\text{-}C_5Me_4H)_2Zr]_2(\mu^2,\eta^2,\eta^2\text{-}N_2)$ and $\{[PhP(CH_2SiMe_2NsiMe_2CH_2]Zr\}_2(\mu^2,\eta^2,\eta^2\text{-}N_2)$ Complexes? A Computational Study“ *J. Am. Chem. Soc.* **2006**, 128 (35), 11391-11403.

181. Yates, B. F.; Basch, H.; Musaev, D. G.; Morokuma, K. „The Reaction of H_2 with a Binuclear Zirconium Dinitrogen Complex- Evaluation of Theoretical Models and Hybrid Approaches“, *J. Chem. Theory and Comput.* **2006,** 2 (5), 1298-1316.

182. Musaev, D. G.; Nowroozi-Isfahani, T.; Morokuma, K.; Abedin, J.; Rosenberg, E.; Hardcastle, K. I. „Experimental and Computational Studies of Nucleophilic Attack, Tautomerization, and Hydride Migration in Benzoheterocycle Triosmium Clusters.“ *Organometallics*, **2006**, 25(1), 203-213.

183. Wang, Y.; Zheng, G.; Morokuma, K.; Geletii, Y. V.; Hill, C. L.; Musaev, D. G. "Density Functional Study of the Roles of Chemical Composition of Di-Transition-Metal-Substituted γ-Keggin Polyoxometalate Anions" *J. Phys. Chem., B* **2006** 110(11); 5230-5237.

184. Prabhakar, R.; Morokuma, K.; Musaev, D. G. " A DFT Study of the Mechanism of Ni Superoxide Dismutase (NiSOD): Role of the Active Site Cysteine-6 Residue in the Oxidative Half-Reaction. *J. Comput. Chem.,* **2006**, 27 (12), 1438-1445.

185. Musaev, D. G.; Xu, S. C.; Irle, S.; Lin, M. C. „The Mechanisms of the Reactions of W and W^+ with H_2O: Computational Studies", *J. Phys. Chem.* A, **2006**, 110(13); 4495-4501

186. Quiñonero, D.; Wang, Y.; Morokuma, K.; Khavrutskii, L. A.; Botar, B.; Geletii, Y. V.; Hill, C. L.; Musaev, D. G. "The role of the central atom in structure and reactivity of polyoxometalates with adjacent d-electron metal sites. Computational and experimental study of γ-$[(X^{n+}O_4)Ru^{III}_2(OH)_2(M_{FM})_{10}O_{32}]^{(8-n)-}$, M_{FM} = Mo and W, and X = Al^{III} Si^{IV}, P^V, and S^{VI}." *J. Phys. Chem., B.* **2006**, *110*, 170-173.

187. Kwiecien, R. A.; Khavrutskii, I. V.; Musaev, D. G.; Morokuma, K.; Banerjee, R.; Paneth, P. "Computational Insights into the mechanism of Radical Generation in B_{12}-Dependent Methylmalonyl-CoA Mutase", *J. Am. Chem. Soc.* **2006**, *128*, 1287-1292.

188. Bobadova-Parvanova, P.; Quinonero-Santiago, D.; Morokuma, K.; Musaev, D. G. Theoretical Study of the Structure and Properties of $[(\eta^5\text{-}C_5Me_4H)_2Zr]_2(\mu^2,\eta^2,\eta^2\text{-}N_2)$. *J. Chem. Theory and Comput.;* **2006;** 2(2); 336-341.

2005

189. Bobadova-Parvanova, Petia; Wang, Qinfang; Morokuma, Keiji; Musaev Djamaladdin, G.; "How many methyl groups in $[\{(\eta^5\text{-}C_5Me_nH_{5-n})_2Zr\}_2(\mu^2,\eta^2,\eta^2\text{-}N_2)$ are needed for dinitrogen hydrogenation? A Theoretical Study" *Angew. Chem. Intern. Ed.* **2005**, 44, 7101-7103

190. Prabhakar R.; Morokuma, K.; Musaev, D. G. „The Computational Approaches to the Enzymes: The Studies of the structure of pyridoxal 5'–phosphate (PLP) dependent *E.coli* NifS CsdB protein." *J. Comput. Chem.* **2005**, 26 (5) 443 – 446.

191. Anderson, T. M.; Cao, R.; Slonkina, E.; Hedman, B.; Hodgson, K. O.; Hardcastle, K. I.; Neiwert, W. A.; Wu, S.; Kirk, M. L.; Knottenbelt, S.; Depperman, E. C.; Keita, B.; Nadjo, L.; Musaev, D. G.; Morokuma, K.; Hill, C. L. "A Palladium-Oxo Complex. Stabilization of this Proposed Catalytic Intermediate by an Encapsulating Polytungstate Ligand" *J. Am. Chem. Soc.* **2005**, *127*, 11948-11949.

192. Ananikov, V. P.; Szilagyi, R.; Morokuma, K.; Musaev, D. G. "Can Steric Effects Induce the Mechanism Switch in the Rhodium-Catalyzed Imine Boration Reaction? A Density Functional and ONIOM Study." *Organometallics*, **2005**, *24*(8), 1938-1946.

193. Xu, S.; Irle, S.; Musaev, D. G.; Lin, M. C. „Water Clusters on Graphite: Methodology for Quantum Chemical *A Priori* Prediction of Reaction Rate Constants" *J. Phys. Chem.* A **2005**, 109, 9563-9572.

194. Ananikov, V. P.; Musaev, D. G.; Morokuma, K. "Theoretical Insight into the C-C Coupling Reactions of the Vinyl, Phenyl, Ethynyl, and Methyl Complexes of Palladium and Platinum." *Organometallics***, 2005**, *24*(4), 715-723.

195. Khavrutskii, I. V.; Musaev, D. G.; Morokuma, K. "Cooperative Pull and Push Effects on the O-O Bond Cleavage in Acylperoxo Complexes of [(Salen)MnIIIL]: Ensuring Formation of Manganese(V) Oxo Species." *Inorganic Chemistry* , **2005**, 44(2), 306-315.

196. Quinonero, D.; Morokuma, K.; Musaev, D. G.; Mas-Balleste, R.; Que, L., Jr.; „Metal-Peroxo versus Metal-Oxo Oxidants in Non-Heme Iron-Catalyzed Olefin Oxidations: Computational and Experimental Studies on the Effect of Water“ *J. Am. Chem. Soc.* **2005;** 127 (18), 6548-6549

197. Nowroozi-Isfahani, T.; Musaev, D. G.; McDonald, F. E.; Morokuma, K. “ Density functional study of Mo-carbonyl catalyzed alkynol cycloisomerization: Comparison with W-catalyzed reaction”, *Organometallics*, **2005**, 24(12), 2921-2929.

198. Musaev, D. G.; Morokuma, K. „Transition Metal Catalyzed □-bond Activation and Formation Reactions“ In: *Topics in Organometallic Chemistry.* Vol: Theoretical Aspects of Transition Metal Catalysis“ Ed: G. Frenking, Wiley, **2005**, 12, 1 – 30

199. Prabhakar, R.; Vreven, T.; Morokuma, K.; Musaev, D. G. „Elucidation of the Mechanism of Selenoprotein Glutathione Peroxidase (GPx) Catalyzed Hydrogen Peroxide Reduction by two Glutathione Molecules: A Density Functional Study“, *Biochemistry,* **2005**, *44*, 11864–11871

200. Musaev, D. G.; Nowroozi-Isfahani, T.; Morokuma, K.; Rosenberg, E. „Computational Studies of the Energetics and Reaction Pathways of Molecular Transformations of Benzoheterocycles on Triosmium Clusters.“ *Organometallics*, **2005**, *24*, 5973-5982.

201. Gonzales, J. M.; Musaev, D. G.; Morokuma, K. „Theoretical Studies of Oxidative Addition of E-E Bonds (E = S, Se and Te) to Pd(0) and Pt(0) Complexes“, *Organometallics*, **2005**, 24. 4908-4914.

202. Anderson, T. M.; Cao, R.; Slokina, E.; Hedman, B.; Hodgson, K. O.; Hardcastle, K. I.; Neiwert, W. A.; Wu, S.; Kirk, M. L.; Knottenbelt, S.; Depperman, E. C.; Musaev, D. G.; Morokuma, K.; Hill, C. L. „A Palladium-Oxo Complex. Stabilization of this Proposed Catalytic Intermediate by and Encapsulating Polytungstate Ligand“*J. Am. Chem. Soc. (Commun.)* **2005,** *127*, 11948-11949.

203. Prabhakar, R.; Li, M.; Musaev, D. G.; Morokuma, K.; Edmondson, D. E. „A Density Functional Theory (DFT) study of the spin forbidden dioxygen activation in Monoamine Oxidase B (MAO B) „ *Flavins and Flavoproteins* **2005**, 127-131.

204. Botar, B.; Geletii, Y. V.; Kogerler, P.; Musaev, D. G.; Morokuma, K.; Weinstock. I. A.; Hill, C. L. “ Asymmetric terminal ligation on substituted sites sites in a disorder-free Keggin anion, [β-$SiFe_2W_{10}O_{36}(OH)_2(H_2O)Cl]^{5-}$ ”, *Dalton Trans.* **2005**, 1-5.

205. Musaev, D. G.; Morokuma, K. „Transition Metal Catalyzed □-bond Activation and Formation Reactions“ In: *Topics in Organometallic Chemistry.* Vol: Theoretical Aspects of Transition Metal Catalysis“ Ed: G. Frenking, Wiley, **2005**, 12, 1 – 30

2004

206. Anderson, T. M.; Neiwert, W. A.; Kirk, M. L.; Piccoli, P. M. B.; Schultz, A. J.; Koetzle, T. F.; Musaev, D. G.; Morokuma, K.; Cao, R.; Hill, C. L. „A Late-Transition Metal-Oxo Complex, $O{=}Pt(H_2O)L_2$, L = $[PW_9O_{34}]^{9-}$ „ *Scienc*e, **2004**, 306 (5704), 2074-2077.

207. Musaev, D. G.; Morokuma, K.; Geletii, Y. V.; Hill, C. L. „ Computational Modeling of di-transition-metal substituted gamma-Keggin Polyoxometalate Anions. Structural Refinement of the protonated divacant lacunary silicodecatungstate“, *Inorg. Chem*. **2004**, 43, 7702 – 7708.

208. Musaev, D. G. „Elucidating the Role of the Pyridoxal 5’- Phosphate (PLP)-dependent b-lyases in Selenocysteine Se-Conjugates Metabolism: A Density Functional Study.“ *J. Phys. Chem. B,* **2004**, 108, 18756 – 18761

209. Prabhakar R.; Musaev, D. G.; Khavrutskii, I. V.; Morokuma, K. „Elucidation of the structure of Glutathione Peroxidase (GPxs) at the ONIOM level“, *J. Phys. Chem B (Letter)* **2004**, 108, 12643-12645.

210. Musaev, D. G. „Theoretical Prediction of a New Dinitrogen Reduction Process: The Utilization of four Dihydrogen Molecules and Zr_2Pt_2 Cluster“, *J. Phys. Chem B* **2004**, 108, 10012-10018.

211. Khavrutskii, I. V.; Musaev, D. G.; Morokuma, K. „Epoxidation of Unfunctionalyzed Olefins by Mn(Salen) Catalyst Using Organic Peracids as Oxygen Source. A Theoretical Study“ “, *Proc. Nat. Acad. Of Sci. (USA)* **2004**, 101, 5743-5748.

212. Khavrutskii, I. V.; Rahim, R. R.; Musaev, D. G.; Morokuma, K. „Axial Ligand as a Mechanistic Switch of the O-O Bond Activation in Acylperoxo Complexes of [(Salen)Mn^{III}L]: Mn^{IV} versus Mn^{V} Oxo Species“, *J. Phys. Chem. B*, **2004**, 108, 3845-3854

213. Geletii, Yu. V.; Musaev, D. G.; Khavrutskii, L.; Hill, C. L. „Peroxynitrite Reactions with Dimethylsulfide and Dimethylselenide: An Experimental Study.“ *J. Phys. Chem. A*, **2004**, 108, 289-294.

214. Musaev, D. G.; Galloway, A. L.; Menger, F. M. „The Roles of Steric and Electronic Effects in the 2-Hydoxy-2'-Nitrodiphenyl Sulfones to 2-(o-Nitrophenoxy)-Benzene-Sulfinic acids Rearrangement(Smiles). Computational Study.“, *J. Molecular Struc (Theochem)*, **2004,** 679, 45-52.

215. Hoffmann, M.; Khavrutskii, I. V.; Musaev, D. G.; Morokuma, K. „The Protein Effects on the O_2 Binding to the Active Site of the Methane Monooxygenase: ONIOM Studies“, *Int. J. Quant. Chem*., **2004**, 99(6), 972-980.

2003

216. Khavrutskii, I. V.; Musaev, D. G**.;** Morokuma, K. „Insights into the Structure and Reactivity of Acylperoxo Complexes in Kochi-Jacobsen-Katsuki Catalytic System. A Density Functional Study“*J. Am. Chem. Soc.* **2003**, 125, 13879-13889.

217. Musaev, D. G.; Hirao, K. „Reactivity of [1,2-benzisotellurazol-3(2H)-one] with the Peroxynitrous Acid: Comparison with their Ebselen Analogues.“ *J. Phys. Chem. A*, **2003,** 107, 9984-9990.

218. Quiñonero, D.; Musaev. D. G.; Morokuma, K. „Theoretical Studies of Non-Heme Iron Catalyst $[(BPMEN)Fe(II)(NCCH_3)_2]^{2+}$ for Olefin Epoxidation and Cis-Dihydroxylation. I. Structures, Stabilities and Electronic Properties of the Catalyst“, *Inorg. Chem*. **2003**, 42, 8449-8455.

219. Khoroshun, D. V.; Inagaki, A.; Suzuki, H.; Vyboishchikov, S. F.; Musaev. D. G.; Morokuma, k. „Versatile and cooperative reactivity of a triruthenium polyhydride cluster. A computational study.“ *J. Am. Chem. Soc.* **2003**, 125(33), 9910-9911.

220. Menger, F. M.; Galloway, A. L.; Musaev, D. G. „Experimental and Computational Support for the Rate/Distance Equation“, *Chem. Comm*. **2003**, 2370-2371.

221. Sakimoto, Y.; Hirao, K.; Musaev, D. G.; „Reactivity of Ebtellur Derivatives with the Peroxynitrite Anion: Comparison with Their Ebselen Analogues“, *J. Phys. Chem. A*, **2003**, 107(29), 5631-5639.

222. Musaev, D. G.; Geletii, Yu. V.; and Hill, C. L. „ Theoretical Studies of the Reaction Mechanisms of Dimethylsulfide and Dimethylselenide with Peroxynitrite.“ *J. Phys. Chem. A*, **2003**, 107(30), 5862-5873.

223. Moc, J.; Musaev, D. G.; Morokuma, K. „ Activation and Adsorption of Multiple H_2 Molecules on Pd_5 Cluster, A Density Functional Study“*J. Phys. Chem. A*, **2003**, 107(24), 4929-4939.

224. Inagaki, A.; Musaev, D. G.; Toshifumi, T.; Suzuki, H.; Morokuma, K. „Skeletal Rearangement in the Trinuclear nido-Ruthenacyclopentadiene Complexes: Theoretical and Experimental Studies“*Organometallics,* **2003**, 22(8); 1718-1727.

225. Musaev, D. G.; Geletii, Yu. V.; Hill, C. L.; Hirao, K. „Can the Ebselen Derivatives Catalyze the Isomerization of Peroxynitrite to Nitrate ? „ *J. Am. Chem. Soc.* **2003**, 125(13), 3877-3888.

226. Ilieva, S.; Galabov, B.; Musaev, D. G.; Morokuma, K. „Computational Study of the Aminolysis of 2-Benzoxazolinone“ , *J. Org. Chem*. **2003**, 68(9), 3406-3412.

227. Musaev, D. G.; Hirao, K. „ The Differences and Similarities in the Reactivity of Peroxynitrite Anion and Peroxynitrous Acid with Ebselen. A Theoretical Study.“ *J. Phys. Chem. A*, **2003**, *107*, 1563-1573.

228. Khavrutskii, I. V.; Musaev, D. G.; Morokuma, K. „ Electronic and NMR Properties of Various Oxo- and Nitrido- Derivatives of $[SalenMn(III)L]^+$, where L=None and Imidazole. A Density Functional Study“ *Inorg. Chem.* **2003**, 42(8); 2606-2621.

229. Khoroshun, D. V.; Warncke, K.; Ke, S.-C.; Musaev, D. G.; Morokuma, K. „Internal degrees of freedom, structural motiffs, and conformational energetics of 5‘-deoxyadenosyl radical: Implications for function in adenosylcobalamin-dependent enzymes. A computational study.“ *J. Am. Chem. Soc.* **2003**, *125(2),* 570-579.

230. Ilieva, S.; Galabov, B.; Musaev, D. G.; Morokuma, K.; Schaefer III, H. F. „Computational Study of the Aminolysis of Esters. The reaction of methylformate with ammonia“ *J. Org. Chem*. **2003**, 68(4); 1496-1502.

2002

231. Musaev, D. G.; Basch, H.; Morokuma, K. „The N≡N Triple Bond Activation by Transition Metal Complexes“, in *Computational Modeling of Homogeneous Catalysis*, Eds. Maseras, F.; Lledos, A., Kluwer Academic Publ., **2002**, 325-361.

232. Sheng, Y.; Musaev, D. G.; Reddy, K. S.; McDonald, F. E.; Morokuma, K. „Computational Studies of Tungsten-Catalyzed Endoselective Cycloisomerization of 4-Pentyn-1-ol“, *J. Am. Chem. Soc*., **2002**, *124*, 4149-4157.

233. Musaev, D. G; Basch, H.; Morokuma, K. „Theoretical Study of the Mechanism of Alkane Hydroxylation and Ethylene Epoxidation Reactions Catalyzed by Diiron Bis-oxo Complexes. The Effect of Substrate Molecules“, *J. Am. Chem. Soc*., **2002**, *124***,** 4135-4148.

234. Basch, H.; Musaev, D. G.; Morokuma, K. „Density functional studies of the electronic and geometric structures of Pt_3^+, Pt_3O^+, $Pt_3O_2^+$ and $Pt_3CH_4^{+\bullet}$, *J. of Molecular Struct. (Theochem)*, **2002**, *586*, 35-46 .

235. Szilagyi, R. K.; Musaev, D. G.; Morokuma, K. "Hydrogen Scrambling in $[(C_5Me_5)Os(dmpm)(CH_3)H]^+$. A Density Functional and ONIOM Study“ *Organometallics*, **2002**, *21*, 555-564.

236. Torrent, M.; Musaev, D. G.; Basch, H.; Morokuma, K. Computational Studies of Reaction Mechanisms of Methane Monooxygenase and Ribonucleotide Reductase. *J. Computational Chem.* **2002**, *23*, 59-76.

237. Khoroshun, D. V.; Musaev, D. G.; Morokuma, K. Is binding energy a measure of interaction strength? Sigma trans promotion effect in transition metal complexes. *Mol. Phys.* **2002**, *100*, 523-532.

238. Ananikov, V. P.; Musaev, D. G.; Morokuma, K. „Vinyl-Vinyl Coupling on Late Transition Metals through C-C Reductive Elimination Mechanism. A Computational Study.“ *J. Am. Chem. Soc*., **2002**, *124***,** 2839-2852.

239. Torrent, M.; Vreven, T.; Musaev, D. G.; Morokuma, K.; Farkas, O.; Schlegel, H. B. "Effect of the Protein Environment on the Structure and Energietcs of Active Sites of Metalloenzymes. ONIOM Study of Methane Monooxygenase and Ribonucleotide Reducrase" *J. Am. Chem. Soc*., **2002**, *124*, 192-193.

2001

240. Ananikov, V. P.; Musaev, D. G.; Morokuma, K. **„**Catalytic Triple Bond Activation and Vinyl-Vinyl Reductive Coupling by Pt(IV) Complexes. A Density Functional Study.“ *Organomettalics*, **2001**, *20*, 1652-1667.

241. Torrent, M.; Musaev, D. G.; Basch, H.; Morokuma, K. „A Density Functional Study of Possible Intermediates of the Reaction of Dioxygen Molecule with Methane Monooxygenase and Ribonucleotide Reductase. II. Water-Assisted Model Studies". *J. Phys. Chem.* B **2001**, *105*, 4453-4463.

242. Basch, H.; Musaev, D. G.; Mogi, K.; Morokuma, K. „A Density Functional Study of the Methane Monooxygenase Catalytic Cycle. Methanol Complex to MMOH Resting State.“ *J. Phys. Chem. B*, **2001**, 105, 8452-8460.

243. Torrent, M.; Mogi, K.; Basch, H.; Musaev, D. G.; Morokuma, K. **„**A Density Functional Study of Possible Intermediates of the Reaction of Dioxygen Molecule with Non-Heme Iron-Complexes. I. N-side versus O-side Mechanism with Water-Free Model.“ *J. Phys. Chem. B*, **2001**, *105*, 8616-8628.

244. Basch, H.; Musaev, D. G.; Mogi, K.; Morokuma, K. Theoretical Studies on Mechanism of the Methane → Methanol Conversion Reaction Catalyzed by Methane Monooxygenase (MMO): The O-side vs N-side Mechanisms. *J. Phys. Chem. A*, **2001**, 105, 3615-3622.

245. Torrent, M.; Musaev, D. G.; Morokuma, K. „The Flexibility of Carboxylate Ligands in Methane Monooxygenase and Ribonucleatide Reductase: A Density Functional Study.“ *J. Phys. Chem.* B **2001**, *105*, 322-327.

246. Szilagyi, R. K.; Musaev, D. G.; Morokuma, K. „Theoretical Studies of Biological Nitrogen Fixation. I. Density Functional Modeling of the Mo-site of the FeMo-cofactor“. *Inorg. Chem.* **2001**, *40*, 766-775.

247. Vyboishchikov, S. F.; Musaev, D. G.; Froese, R. J. D.; Morokuma, K. „Density Functional Study of Ethylene Polymerization Catalyzed by Zirconium Non-Cyclopentadienyl Complex, $L_2ZrCH_3^+$. Effects of Ligands and Bulky Substituents.“ *Organometallics*, **2001**, *20*, 309-323.

248. Morokuma, K.; Musaev, D. G.; Vreven, T.; Basch, H.; Torrent, M.; Khoroshun, D. V.; **„**Modeling Reactivities of Metalloenzymes- Studies on Simple Model Enzymes and New Tool for More Realistic Models.“ *IBM Journal Res. & Develop.* **2001**, *45*, 3/4, 367-395.

249. Khoroshun, D. V.; Musaev, D. G.; Vreven, T.; Morokuma, K. **„**Theoretical Study on Bis(imino)pyridyl-Fe(II) Olefin Poly- and Oligomerization Catalysts. Dominance of Different Spin States in Propagation and β-hydride Transfer Pathways.“ *Organometallics*, **2001**, 20, 2007-2026.

2000

250. Matsubara, T.; Koga, N.; Musaev, D. G.; Morokuma, K. „Density Functional Study on Highly Ortho Selective Addition of Aromatic CH Bond to Olefin Catalyzed by $Ru(H)_2(CO)(PR_3)_2$ Complex.“ *Organometallics***, 2000**, *19*, 2318-2329.

251. Moc, J.; Musaev, D. G.; Morokuma, K. „Adsorption of Multiple H_2 Molecules on Pd_3 and Pd_4 clusters. A Density Functional Study.“ *J. Phys. Chem*. A, **2000**, *104*, 11606-11614.

252. Basch, H.; Musaev, D. G.; Morokuma, K. „Can the Binuclear Dinitrogen Complex $[P_2N_2]Zr(\mu–\eta^2–N_2)Zr[P_2N_2]$ Activate More Than One Hydrogen Molecule? A Theoretical Study,“ *Organometallics*, **2000,** *19,* 3393-3403.

253. Torrent, M.; Musaev, D. G.; Morokuma, K. „Theoretical Study of the Mechanism of Oxidative Addition of Allyl-Ammonium and -Iminium Salts to Low-Valent Metal Complexes. Rationalization of Selective C-N and N-H Bond Activation,“ *Organometallics*, **2000**, *19(21),* 4402-4415

254. Szilagyi, R. K.; Musaev, D. G.; Morokuma, K. „Theoretical Studies of Biological Nitrogen Fixation II. Hydrogen Bonded Networks as Possible Reactant and Product Channels.“ *J. Molecular Structure (THEOCHEM),* **2000**, *506*, 131-146.

1999

255. Basch, H.; Mogi, K.; Musaev, D. G.; Morokuma, K. Mechanism of the Methane → Methanol Conversion Reaction Catalyzed by Methane Monooxygenase: A Density Functional Study. *J. Am. Chem. Soc*. **1999**, *121,* 7249-7256**.**

256. Basch, H.; Musaev, D. G.; Morokuma, K. Why Does the Reaction of the Dihydrogen Molecule with $[P_2N_2]Zr(\mu–\eta^2\text{-}N_2)Zr[P_2N_2]$ Produce $[P_2N_2]Zr(\mu–\eta^2\text{-}N_2H)Zr[P_2N_2](\mu\text{-}H)$ but Not the Thermodynamically More Favorable $[P_2N_2]Zr(\mu\text{-}NH)_2Zr[P_2N_2]$? A Theoretical Study. *J. Am. Chem. Soc*., **1999**, *121*, 5754-5761**.**

257. Khoroshun, D. V.; Musaev, D. G.; Morokuma, K. Does Reaction of Three-Coordinate Molybdenum(III) with N_2O Proceed via the same Mechanism as with N_2 ? A Theoretical Study. *Organometallics*, **1999**, *18*, 5653-5660.

258. Torrent, M.; Musaev, D. G.; Ke, S.-C; Warncke, K.; Morokuma, K. Calculation of Nuclear Quadrupole Parameters in Imidazole Derivatives and Extrapolation to Coenzyme B_{12}. A. Theoretical Study. *J. Phys. Chem.* B. **1999**, *103*, 8618-8627

259. Ke, S.-C.; Torrent, M.; Musaev, D. G.; Morokuma, K.; Warncke, K. Identification of Dimethylbenzimidazole Axial Coordination and Characterization of ^{14}N Superhyperfine and Nuclear Quadrupole Coupling in Cob(II)alamin Bound to Ethanolamine Deaminase in a Catalytically-Engaged Substrate Radical-Cobalt(II) Biradical State. *Biochemistry*, **1999**, 38, 12681-12689

260. Musaev, D. G.; Morokuma, K. Theoretical Studies of the Mechanism of Ethylene Polymerization Reaction Catalyzed by Diimine-M(II) (M=Ni, Pd and Pt) and Ti- and Zr-Chelating Alkoxides.*Topics in Catalysis*, **1999**, 7, 107-123.

261. Bandrauk, A. D.; Musaev, D. G.; Morokuma, K. Electronic States of the Triply Charged Molecular ion N_2^{3+} and Laser-Induced Coulomb Explosion. *Phys. Rev*. A. **1999**, 59, 4309-4315.

262. Bacalzo-Gladden, F. T.; Musaev, D. G.; Lin, M. C. “A Model Calculation for the Isomerization and Decomposition of Chemisorbed HCN on the Si(100)-2x1 Surface.” *J. Chin. Chem. Soc.* **1999**, *46*, 395-402.

263. Froese R. D. J.; Musaev, D. G.; Morokuma, K. Theoretical Studies of the Factors Controlling Insertion Barriers for Olefin Polymerization by the Ti-Chelating Bridged Catalysts. The Search for More Active New Catalysts. *J. Am. Chem. Soc,* **1999**, 18, 373-379

264. Musin, R. N.; Musaev, D. G.; Lin, M. C. "Quantum Chemical Study of the Structure and Properties of Hypothetical Superhard Materials Based on the Cubic Silicon-Carbon Nitrides," *J. Phys. Chem.* B, **1999**, 103, 797-803.

265. Basch, H.; Musaev, D. G.; Morokuma, K.; Fryzuk, M. D.; Love, J. B.; Seidel, W. S.; Albinati, A.; Koetzle, T.; Klooster, W. T.; Mason, S. A.; Eckert, J. Theoretical Predictions and Single Crystal Neutron Structural Study on the Reaction of Dihydrogen with the Dinuclear Dinitrogen Complex of Zirconium $[P_2N_2]Zr(\mu-\eta^2-N_2)Zr[P_2N_2]$, P_2N_2 = $PhP(CH_2SiMe_2NSiMe_2CH_2)_2PPh$, *J. Am. Chem. Soc.,* **1999,** *121*, 523-528.

266. Froese R. D. J.; Musaev, D. G.; Morokuma, K. Theoretical Studies of the Cp_2ZrR^+-Catalyzed Propylene Polymerization Reactions and a Comparison with Ethylene Polymerization, *J. of Molecular Structure (THEOCHEM),* **1999,** 461-462, 121-135.

267. Musaev, D. G.; Cui, Q.; Svensson, M.; Morokuma, K. Theoretical Studies of the N_2 Cleavage by Three-Coordinate Group 6 Complexes ML_3. In American Chemical Society series, "*Transition State Modeling for Catalysis*", Ed. Truhlar, D. G. ; Morokuma, K. ; ASC Symposium series, ACS, Washington DC, **1999**, 198-207.

268. Das, P. K.; Dockter, D. W.; Fahey, D. R.; Lauffer, D. E.; Hawkins, G. D.; Li, J.; Zhu, T.; Cremer, C. J.; Truhlar, D. G.; Dapprich, S.; Froese, R. D. J.; Holtahusen, M. C.; Liu, Z.; Mogi, K.; Vybroschikov, S.; Musaev, D. G.; Morokuma, K. Ethylene Polymerization by Zirconocene Catalysts, In American Chemical Society Series, "*Transition State Modeling for Catalysis*", Ed. Truhlar, D. G.; Morokuma, K.; ASC Symposium series, ACS, Washington DC, **1999**, 208-225.

1998

269. Matsubara, T.; Koga, N.; Musaev, D. G.; Morokuma, K. Density Functional Study on Activation of ortho-CH Bond in Aromatic Ketone by Ru-Complex. Role of Unusual Five-Coordinated d^6 Metallacycle Intermediate with Agostic Interaction *J. Am. Chem. Soc.,* **1998,** 120 (48), 12692 — 12693.

270. Yandulov, D. V.; Caulton, K. G.; Belkova, N. V.; Shubina, E. S.; Epstein, L. M.; Khoroshun, D. V.; Musaev, D. G.; Morokuma, K. Diminishing π–Stabilization of an Unsaturated Metal Center: Hydrogen Bonding to $OsHCl(CO)(P_tBu_2Me)_2$, *J. Am. Chem. Soc.,* **1998**, 120, 12553-12563.

271. Cui, Q.; Musaev, D. G.; Morokuma, K. Molecular Orbital Study of H_2 and CH_4 activation on small metal clusters. I. Pt, Pd, Pt_2 and Pd_2. *J. Chem. Phys.,* **1998**, 108, 8418-8428.

272. Cui, Q.; Musaev, D. G.; Morokuma, K. Molecular Orbital Study of H_2 and CH_4 activation on small metal clusters. I. Pt_3 and Pd_3. *J. Phys. Chem, A* **1998**, 102, 6373-6384.

273. Musaev, D. G.; Froese, R. D. J.; Morokuma, K. Molecular Orbital and IMOMM Studies of the Chain Transfer Mechanisms of the Diimine-M(II) (M=Ni and Pd) Catalyzed Ethylene Polymerization Reaction. *Organometallics,* **1998**, 17, 1850-1860.

274. Johnson A. R.; Davis, W. M.; Cummins, C. C.; Serron S.; Nolan, S. P.; Musaev, D. G.; Morokuma, K. Four-Coordinate Molybdenum Chalocogenide Complexes Relevant to Nitrous Oxide N-N Bond Cleavage by Three-Coordinate Molybdenum (III): Synthesis, Characterization, Reactivity, and Thermochemistry. *J. Am. Chem. Soc.,* **1998**, 120, 2071-2085.

275. Cui, Q.; Musaev, D. G.; Morokuma, K. Density Functional Study of the Mechanism of Pd(0)-Catalyzed Thioboration Reaction of Alkynes. Differences between Pd(0)- and Pt(0)-Catalysts and between Thioboration and Diboration. *Organometallics,* **1998**, 17, 1383-1392.

276. Bacalzo, F. T.; Musaev, D. G.; Lin, M.C. **"**Theoretical Studies of CO Adsorption on Si(100)-2x1 Surface." *J. Phys. Chem.* **1998**, 102, 2221-2225

277. Cardelino B. H.; Moore C. E.; Frazier D. O.; Musaev, D. G.; Morokuma, K. Ab Initio Calculations on the Diacetylene Dimer: HCCCC(H)CCCH. *Int. J. Quantum Chemistry* **1998**, 66, 189-202.

278. Froese R. D. J.; Musaev, D. G.; Morokuma, K. A Theoretical Study of Substituent Effects in the Diimine-M(II) Catalyzed Ethylene Polymerization Reaction Using the IMOMM Method. *J. Am. Chem. Soc.* **1998**, 120, 1581-1587.

279. Cui, Q.; Musaev, D. G.; Morokuma, K. **"**Why Do $Pt(PR_3)_2$ Complex Catalyze the Alkyne Diboration Reaction, But Their Pd Analogs Do Not ? A Density Functional Study." *Organometallics,* **1998**, 17, 742-751.

1997

280. Froese, R. D. J.; Musaev, D. G.; Matsubara, T.; Morokuma, K. Theoretical Study of the Ethylene Polymerization Reactions Catalyzed by Zirconium and Titanium Chelating Alkoxide Complexes, *J. Am. Chem. Soc.* **1997**, 119, 7190.

281. Musaev, D. G.; Froese, R.D.J.; Morokuma, K. Transition Metal Catalyzed Olefin Polymerization Reaction: Comparison of the Mechanism of the Dimine-M(II) (M= Ni and Pd) and Zirconocene-based Processes. *New J. Chem.,* **1997**, 21, 1269-1282.

282. Musaev, D. G.; Svensson, M.; Morokuma, K.; Stromberg, S.; Zetterberg, K.; Siegbahn, P. E. M. "A Density Functional Study of the Mechanism of the Diimine-Pd(II)-Catalyzed Ethylene Polymerization Reaction." *Organometallics,* **1997**, 16, 1933.

283. Cui, Q.; Musaev, D. G.; Morokuma, K. The Studies of the Mechanism of Pt(0)-Catalyzed Alkene and Alkyne Diboration Reactions. *Organometallics,* **1997**, 16, 1355.

284. Matsubara, T.; Koga, N.; Ding, Y.; Musaev, D. G.; Morokuma, K. Ab Initio MO Study of the Full Catalytic Cycle of Olefin Hydroformylation by Rhodium Complex $RhH(CO)_2(PH_3)_2$. *Organometallics,* **1997**, 16, 1065.

285. Cini, R.; Musaev, D. G.; Marzilli, L. G.; Morokuma, K. A Molecular Orbital Study of Complexes of Zinc(II) with Imidazole and Water Molecules. *J. Molecular Structure (THEOCHEM),* **1997,** 392, 55.

286. Musaev, D. G.; Froese, R. D. J.; Svensson, M.; Morokuma, K. A Density Functional Study of the Mechanism of the Diimine-Nickel-Catalyzed Ethylene Polymerization Reaction. *J. Am. Chem. Soc.* **1997**, 119, 367.

1996

287. Wu, G.; Rovnyak, D.; Johnson, M. J. A.; Zanetti, N. C.; Musaev, D. G.; Morokuma, K.; Schrock R. R.; Griffin, R. G.; Cummins, C. C. Unusual ^{31}P Chemical Shielding Tensors in Terminal Phosphido Complexes Containing a Phosphorus-Metal Triple Bond. *J. Am. Chem. Soc.* **1996**, 118, 10654.

288. Dapprich S.; Ujaque G.; Maseras F.; Lledos A.; Musaev, D. G.; Morokuma, K. Theory Does Not Support an Osmaoxetane Intermediate in the Osmium-Catalyzed Dihydroxylation of Olefins. *J. Am. Chem. Soc.* **1996**, 118, 11660.

289. Musaev, D. G.; Morokuma, K. Potential Energy Surfaces of Transition Metal Catalyzed Chemical Reactions. *Adv. Chem. Phys.* **1996**, p.61-128 (**Review**).

290. Musaev, D. G.; Morokuma, K. The Structure, Stability and Bonding of Transition Metal-Boryl Complexes. A Molecular Orbital Study. *J. Phys. Chem.,* **1996**, 100, 6509.

291. Musaev, D. G.; Morokuma, K. Molecular Orbital Study of the Reaction Mechanism of Sc^+ with Methane. Comparison of the Reactivity of Early and Late First Row Transition Metal Cations and Their Carbene Complexes. *J. Phys. Chem.,* **1996**, 100, 11600.

292. Cui, Q.; Musaev, D. G.; Svensson, M.; Morokuma, K. Analytical Second Derivatives For Effective Core Potential. Application to Transition Structures of $Cp_2Ru_2(\mu\text{-}H)_4$ and to the Mechanism of Reaction Cu + CH_2N_2 . *J. Phys. Chem.* **1996**, 100, 10936.

293. Morokuma, K.; Yoshida, T.; Koga, N.; Musaev, D. G. Combined MO + MM theoretical studies on isotacticity control in propylene polymerization with group 4 metallocenes**.** *Polym. Mater. Sci. Eng.* **1996**, *74*, 425.

1995

294. Cui, Q.; Musaev, D. G.; Svensson, M.; Sieber, S.; Morokuma, K. "N_2 Cleavage by Three-Coordinate Group 6 Complexes. W(III) Complexes Would be Better Than Mo(III) Complexes." *J. Am. Chem. Soc.* **1995**, 117, 12366.

295. Musaev, D. G.; Morokuma, K. Ab Initio Molecular Orbital Study of Oxidative Addition of H_2 and CH_4 to $RhCl(CO)(PH_3)_2$ Complex. *J. Organomet. Chem.* **1995**, 504, 93.

296. Gazdy, B.; Musaev, D. G.; Bowman, J. M.; Morokuma, K. An Ab Initio Study of the ground and first excited state of HCN $\leftrightarrow$ HNC Isomerization and a calculation of the HNC A $\rightarrow$ X Fluorescence Spectrum. *Chem. Phys. Lett.* **1995**, 237, 27.

297. Musaev, D. G.; Morokuma, K. Does tetrahydroborane species $AuBH_4$ exist? Ab initio MO study of the structure and stability of the $CuBH_4$, $AgBH_4$ and $AuBH_4$. *Organometallics* **1995**, 14, 3327.

298. Musaev, D. G.; Morokuma, K. Ab Initio Molecular Orbital Study of the Mechanism of H-H, C-H, N-H, O-H and Si-H Bonds activation on Transient Cyclopentadienylcarbonylrhodium. *J. Am. Chem. Soc.* **1995**, 117, 799.

299. Musaev, D. G.; Matsubara, T.; Mebel, A. M.; Koga, N.; Morokuma, K. Ab Initio Molecular Orbital Studies of Elementary Reactions and Homogeneous Catalytic Cycles with Organometallic Compounds. *Pure and Applied Chem.* **1995**, 67, 257-263.

1994

300. Musaev, D. G.; Morokuma, K. Ab Initio Molecular Orbital Study of The Molecular and Electronic Structure of $FeCH_2^+$ and of The Reaction Mechanism of $FeCH_2^+ + H_2$. *J. Chem. Phys.* **1994**, 101, 10697

301. Reihl, J.-F.; Musaev, D. G.; Morokuma, K. An ab initio Molecular Orbital Study of the Unimolecular Dissociation Reactions of di- and trichloroethylene. *J. Chem. Phys.*, **1994**, 101, 5942

302. Musaev, D. G.; Mebel, A. M.; Morokuma, K. An ab initio Molecular Orbital Study of Mechanism of the Rhodium(I)-Catalyzed Olefin Hydroboration Reaction. *J. Am. Chem. Soc.* **1994**, 116, 10693-10702.

303. Mebel, A. M.; Musaev, D. G.; Morokuma, K. Ab Initio MO Study of Skeletal Rearrangements in Pentagonal Pyramidal Clusters, B_6H_{10} Borane and $[(IrB_5H_8)(CO)(PH_3)_2]$ Metalloborane. *J. Am. Chem. Soc.* **1994**, 116, 3932-3942.

1993

304. Mebel, A. M.; Musaev, D. G.; Koga, N.; Morokuma, K. Metalloboranes with VIIIB subgroup transition metals. Is accurate ab initio molecular orbital calculation of structure, stability and NMR chemical shifts possible? *Bull. Chem. Soc. Jpn*, **1993**, 66, p.3259-3270.

305. Mebel, A. M.; Musaev, D. G.; Morokuma, K. An alternative mechanism of BH_2SH formation in the reaction of B_2H_6 with SH_2: Concerted elimination of BH_3 and H_2 from $H_2S.B_2H_6$. Ab initio MO study. *Chem. Phys. Lett.* **1993**, 216, 313-318.

306. Mebel, A. M.; Musaev, D. G.; Morokuma, K. Ab initio molecular orbital study of structure and NMR ^{11}B chemical shifts of Lewis base adducts of CO, NH_3, CO, PF_3 and PH_3 with small nido-boranes, B_3H_7 and B_4H_8. *Chem. Phys. Lett.* **1993**, 214, 69-76.

307. Musaev, D .G.; Morokuma, K.; Koga, N. Ab initio Molecular Orbital Study of Electronic and Geometrical Structure of MCH_2^+ and $MSiH_2^+$ Complexes (M = Co, Rh and Ir). *J. Chem. Phys.* **1993**, 99, 7859-7872.

308. Musaev, D. G.; Morokuma, K. Ab Initio Molecular Orbital Study of the Electronic and Geometrical Structure of MCH_2^+ and Reaction Mechanism: $MCH_2^+ + H_2 \rightarrow M^+ + CH_4$. (M = Co, Rh and Ir). *Isr. J. Chem.,* **1993**, 33, 307-316.

309. Mebel, A. M.; Musaev, D. G.; Morokuma, K. Ab Initio Molecular Orbital Study of Mechanisms of Reaction of B_2H_6 with SH_2. *J. Phys. Chem.,* **1993**, 97, 7543 - 7552.

310. Musaev, D. G.; Morokuma, K.; Koga, N.; Nguyen, K. A.; Gordon, M. S.; Cundari, T. R. An Ab Initio Study of the Molecular and Electronic Structure of $CoCH_2^+$ and The Reaction Mechanism: $CoCH_2^+ + H_2$. *J. Phys. Chem.,* **1993**, 97, 11435-11444.

311. Musaev, D. G.; Koga, N.; Morokuma, K. Ab initio Molecular Orbital Study of the Electronic and Geometrical Structure of RhCH2+ and The Reaction Mechanism: $RhCH_2^+ + H_2 \rightarrow Rh^+ + CH_4$. *J. Phys. Chem.,* **1993,** 97, 4064 - 4075.

From USSR: 1992 – 1981

312. Zyubin, A. S.; Musaev, D. G.; Charkin, O. P. A theoretical study of the relative stability of the trigonal prismatic and octahedral structures of six-coordinate compounds MX_6. *Russ. J. Inorg. Chem*. **1992**, v. 37(10), p. 1214-1219.

313. Musaev, D. G.; Geskin, V. M.; Yacobson, V. V.; Charkin, O. P. Theoretical study of the effect of cations Li^+, Na^+ and Cu^+ on the isomerism of HCN ↔ CNH. *Zh. Neorg. Khim.,* **1991**, v.36, N 11, p.2889-2894.

314. Musaev, D. G.; Yacobson, V. V.; Charkin, O. P. Theoretical study of structure and stability of Li_2BO^+, Li_2AlO^+, Li_2BS^+ and Li_2AlS^+. *Zh. Neorg. Khim.,* **1991**, v.36, N 9, p.2340-2350.

315. Zyubin, A. S.; Musaev, D. G.; Charkin, O. P. Ab initio MO study of the structures and stability of complex hydrides LB_2H_7, LBAlH7 and LAl2H7 (L= Li+, Na+ and Cu+). *Zh. Neorg. Khim.,* **1991**, v.36, N 9, p.2330-2339.

316. Musaev, D. G.; Charkin, O. P. Nonempirical studies of structures and stability of boro- and alumo-hydrides of K, Ca, Cu and Zn. *Zh. Neorg. Khim.,* **1991,** v.36, N 3, p.760-764.

317. Musaev, D. G.; Yacobson, V. V; Charkin, O. P. Theoretical study of isomerism: $(H_2OLi)^+AB \rightarrow (H_2OLi)^+BA$ (AB = CO, NP, CN^-, BO^-, CP^-, SiN^- and SiP^-). *Zh. Neorg. Khim.,* **1991**, v.36, N 1, p.72-77.

318. Musaev, D. G.; Charkin, O. P. Theoretical study of structure and stability of the species $LiBH_2$-$LiAlH_2$-$LiScH_2$ and $CuBH_2$-$CuAlH_2$-$CuScH_2$. *Zh. Neorg. Khim.,* **1991**, v.36, N 6, p.1267-1278.

319. Musaev, D. G.; Charkin, O. P. Theoretical study of structure and stability of the molecules $CuBO_2$, CuOBS, $CuBS_2$, $CuAlO_2$, CuOAlS and $CuAlS_2$. *Zh. Neorg. Khim.,* **1991**, v.36, N 3, p.456-465.

320. Musaev, D. G.; Yacobson,V. V.; Charkin, O. P. Theoretical study of the isomerism in the HAB → ABH (AB= BO^-, CO, CN^-, BS^-, CS, CP-, AlO, SiN^-, AlS-, SiS and SiP^-).*Zh. Strukt. Khim.,* **1991**, v.32, N 3, p.11-30.

321. Musaev, D. G.; Charkin, O. P. Theoretical study of the isomerism in the molecules CuCNS and CuNCS. *Koord. Khim.,* **1991,** v.17, N 5, p. 680-689.

322. Musaev, D. G.; Yacobson, V. V.; Charkin, O. P. Theoretical study of the structure and stability of the ion-molecular complexes Li^+CO_2, Li^+OCS, Li^+CS_2, Li^+SiO_2, Li^+OSiS and Li^+SiS_2. *Zh. Strukt. Khim.,* **1990**, v.35, N 3, p.704-710.

323. Musaev, D. G. Theoretical study of the structure and stability of the ion-molecular clusters $NH_4^+(H_2)_n$ and $NH_4^+(N_2)_n$. *Zh. Neorg. Khim.,* **1990**, v.35, N 6, p. 1464-1470.

324. Musaev, D. G.; Makhaev, V. D.; Charkin, O.P. Theoretical study of structure and stability of the complexes $Cu^+(H_2)_n$ (n=1-4) and LCu^+H_2 (L = CO, N_2, H_2O, NH_3, CN^- and BH_4^-). *Koord. Khim.,* **1990**, v.16, N 6, p. 749-757.

325. Musaev, D. G.; Charkin, O. P. Theoretical study of structure and stability of the complexes Cu^+ with molecules H_2, CH_4 and C_2H_6. *Zh. Neorg. Khim.,* **1990**, v.35, N 3, p.689-698.

326. Musaev, D. G.; Charkin, O. P. Theoretical study of structure and stability of the ion-molecular clusters $Be^{2+}(H_2)_n$ (n = 1-6). *Zh. Strukt Khim.,* **1990**, v.31, N 2, p.18-29.

327. Musaev, D. G.; Yacobson, V. V.; Charkin, O. P. Theoretical study of the structure and stability of the molecules $LiBO_2$, LiOBS, $LiBS_2$, $LiAlO_2$, LiOAlS and $LiAlS_2$. *Zh. Neorg. Khim.,* **1989,** v.34, N 8, p.1946-1952.

328. Musaev, D. G.; Charkin, O. P. Theoretical study of the structure and stability of ion-molecular complexes $(H_2O)_nBe^{2+}(H_2)_m$. *Zh. Neorg. Khim.,* **1989,** v.34, N 6, p.1372-1378.

329. Yacobson, V. V.; Musaev, D. G.; Zyubin, A. S.; Mebel, A. M.; Charkin, O. P. Theoretical study of the Li^+ affinity of the hydrides MH_n, fluorides MF_n and lithides MLi_n molecules. *Koord. Khim.,* **1989,** v.15, N 11, p. 1478-1488.

330. Musaev, D. G.; Mebel, A. M.; Charkin, O. P.; Cimiraglia, R.; Tomasi, J. Nonempirical study of isomerism in the CuOAl and CuCP molecules using pseudopotential method. *Koord. Khim.,* **1989**, v.15, N 9, p. 1155-1161.

331. Musaev, D. G.; Yacobson, V. V.; Charkin, O. P. Theoretical study of isomerism in the LiNCS and LiCNS molecules. *Koord. Khim.,* **1989,** v.15, N 8, p. 1011-1021.

332. Musaev, D. G.; Yacobson, V. V.; Charkin, O. P. Theoretical study of isomerism in carbonil fragments LCO-->COL (L = Li^+, Be^{2+}, HLi, FLi, LiLi, H_2Li^-). *Koord. Khim.,* **1989**, v.15, N 5, p. 588-599.

333. Musaev, D. G.; Charkin, O. P. Theoretical study of structure and stability of complexes of the molecular hydrogen with the K^+, Cu^+, Be^{2+} and Zn^{2+} ions. *Zh. Strukt. Khim.,* **1989**, v.30, N 3, p.11-18.

334. Yacobson, V. V.; Musaev, D. G.; Charkin, O. P. Theoretical study of the isomerism in the salts and ion-molecular complexes of Li such as Li^+AB (AB= SiN^-, AlO^-, SiP^-, AlS^-, SiO, AlF, P_2 and AlCl). *Zh. Strukt. Khim.,* **1989**, v.30, p.19-28.

335. Musaev, D. G.; Charkin, O. P. Nonempirical study of the structure and stability of the 3d-transition metal hydrides MH_k, MH_{k+1}^- and MH_{k-1}^+. *Koord. Khim.,* **1989**, v.15, N 2, p. 161-169.

336. Musaev, D. G. Theoretical study of isomeric rearrangement in complexes with homonuclear frameworks of the nitrogen and phosphorus. *Zh. Neorg. Khim.,* **1988,** v.33, N 12, p. 3207-3210.

337. Musaev, D. G.; Charkin, O. P. Nonempirical study of the structure and stability of 3d-transition metal fluorides MF_k and MF_{k+1}^- *Koord. Khim.,* **1988**, v.14, N 11, p. 1460-1467.

338. Yacobson, V. V.; Musaev, D. G.; Charkin, O. P. Theoretical study of the isomerism in the molecules of the salts and ion-molecular complexes of Li_2AB^+ (AB = CP^-, BS^-, NP, CS and BCL). *Zh. Strukt. Khim.,* **1988,** v. 29, N 4, p. 3-10.

339. Musaev, D. G.; Zyubin, A. S.; Charkin, O. P.; Bonaccorsi, R.; Tomasi, J. Theoretical study of the structure and stability of diborane, hexahydro-aluminum-boran and hexa-hydro-boran scandium. *Koord. Khim.,* **1988**, v.14, N 5, p. 638-647.

340. Zyubin, A. S.; Musaev, D. G.; Charkin, O. P. Nonempirical calculations of the structure and stability of group II element borohydrides of the type $HLiBH_4$ and $L(BH_4)_2$. *Koord. Khim.,* **1987**, v.13, N 10, p. 1329-1339.

341. Musaev, D. G.; Yacobson, V. V.; Klimenko, N. M.; Charkin, O. P. Theoretical study of isomersm in salts and ion-molecular complexes of Cu(I). *Koord. Khim.,* **1987**, v.13, N 9, p. 1188-1197.

342. Charkin, O. P.; Bonaccorsi, R.; Tomasi, J.; Zyubin, A. S.; Musaev, D. G. Nonempirical MP_4 calculations of structure and stability of the calcium borohydrides. *Zh. Neorg. Khim.,* **1987**, v.32, N 12, p. 2907-2910.

343. Yacobson, V. V.; Musaev, D. G.; Charkin, O. P. Ab initio CI study of the isomerism of lithium salts and ion-molecule complexes Li+AB → ABLi+ (AB = CN-, BO-, BeF-, N2, CO, BF). *Zh. Strukt. Khim.,* **1986**, v.27, N 6, p.18-30.

344. Klimenko, N. M.; Musaev, D. G.; Gorbik, A. A.; Zyubin, A. S.; Charkin, O. P.; Wuthwein, E. U.; Schleyer, P.v.R. Nonempirical calculations of the structure and stability of lithium clusters ALi_{2k} of the second group elements. *Koord. Khim.,* **1986,** v.12, N 5, p. 601-607.

345. Klimenko, N. M.; Musaev, D. G.; Charkin, O. P. Nonempirical investigation of simple comounds of 3d-metals. *Zh. Struct. Khim.,* **1985**, v. 26, N 5, p. 3-11.

346. Charkin, O. P.; Musaev, D. G.; Klimenko, N. M. Theoretical study of stability and structure of the complex hydrides LBH_4 and $LiMH_4$ (L = Li, Na, K and Cu, M = B, Al and Sc). *Koord. Khim.,* **1985**, v.11, N 6, p. 728-733.

347. Charkin, O. P.; Musaev, D. G.; Klimenko, N. M. Nonempirical study of isomerism in molecules LCN cyanides and L^+CO carbonyls (L = Li, Na, K, Cu). *Koord. Khim.,* **1985**, v.11, N 4, p. 445-456.

348. Musaev, D. G.; Boldyrev, A. I.; Charkin, O. P.; Klimenko, N. M. Ab initio study of the isomerism in CuCN molecule. *Koord. Khim.,* **1984**, v.10, p. 938-941.

349. Klimenko, N. M.; Musaev, D. G.; Zyubina, T. S.; Charkin, O. P. Nonempirical study of isomerism in molecules XOSc and XOCu (X= H, Li and F). *Koord. Khim.,* **1984**, v.10, N 4, p. 505-510.

350. Musaev, D. G.; Boldyrev, A. I. Ab initio investigation of inversion in molecules TiX_4 and ScX_4^- (X= H and F). *Koord. Khim.,* **1984,** v.10, N 3, p. 309- 312.

351. Klimenko, N. M.; Musaev, D. G.; Charkin, O. P. Theoretical studies of the geometry of difluorides of 3d- metals. *Zh. Neorg. Khim.*, **1984**, v. 29, N 5, p. 1114-1116.

352. Klimenko, N. M.; Musaev, D. G.; Charkin, O. P. Theoretical studies of the geometry of triatomic oxides and oxo-fluorides of 3d- metals. *Zh. Neorg. Khim.*, **1984**, v. 29, N 4, p. 835-838.

353. Klimenko, N. M.; Musaev, D. G.; Zyubin, A. S. Possibility of nonempirical MO LCAO SCF calculations with the middle basis sets of the molecule transition 3d- metals. *Zh. Neorg. Khim.*, **1984,** v. 29, N 3, p. 607-609.

354. Musaev, D. G.; Borisov, Yu. A. Calculations of molecules with floating sherical Gaussian Orbital (FSGO) method. II. Complexes of molecules H_2, CO, N_2 and H_2O with the lithium cation. *Zh. Strukt. Khim.*, **1982**, v. 23, N 4, p. 20-24.

355. Musaev, D. G.; Borisov, Yu. A. Calculations of molecules with floating sherical Gaussian Orbital (FSGO) method. I. Simple molecules and ions. *Zh. Strukt. Khim.*,**1982**, v. 23, N 1, p. 10-15.

356. Musaev, D. G.; Borisov, Yu. A. Calculation of matrix elements of the pseudopotential operator by using gaussian functions. *Zh. Strukt. Khim.*, **1981**, v. 22, N 1, p. 169-170.