

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

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2009

1. A. E. Kuznetsov, Y. V. Geletii, C. L. Hill, K. Morokuma, D. G. Musaev, „Mechanism of the Divanadium-Substituted Polyoxotungstate $[g\text{-}1,2\text{-H}_2\text{SiV}_2\text{W}_{10}\text{O}_{40}]^{4-}$ Catalyzed Olefin Epoxidation by H_2O_2 : A Computational Study“, *Inorg. Chem.* **2009**, *48*, 1871-1878
2. Aleksey E. Kuznetsov, Djamaladdin G. Musaev, „ Does the MgO(100)-support facilitate the reaction of dinitrogen and dihydrogen molecules catalyzed by Zr_2Pd_2 Clusters? A Computational Study“, *J. Phys. Chem. C*, **2009**, *submitted*
3. 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**, in press.
4. 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, $g\text{-}[\text{XW}_{10}\text{O}_{38}\{\text{RuN}\}_2]^{6-}$ (X=Si or Ge)“, *Eur. J. Chem.* **2009**, in press
5. 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
6. David Quinero, Djamaladdin G. Musaev, Keiji Morokuma, „Computational insights to the mechanism of alkene epoxidation by manges-based catalysts in the presence of bicarbonate“, *J. Molecular Structure: THEOCHEM*, **2009**, *903(1-3)*, 115-122
7. A. E. Kuznetsov, Y. V. Geletii, C. L. Hill, K. Morokuma, D. G. Musaev, „ 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
8. 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 $[\text{RhCl}_3(\text{SbPh}_3)_3]^-$ “, *Polyhedron*, **2009**, in press
9. 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.
10. 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
11. 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
12. Rui Cao, Travis M. Anderson, Kenneth I. Hardcastle, Djamaladdin G. Musaev, Keiji Morokuma,

Craig L. Hill, „A Dinuclear Terminal Palladium-oxo Complex: $\text{Cs}_{3.5}\text{K}_3\text{Na}_{3.5}[(\text{O}=\text{Pd}^{\text{IV}}(\text{OH}_2))_2\text{P}_2\text{W}_{19}\text{O}_{69}(\text{OH}_2)]$ “, *J. Am. Chem. Soc.*, **2009**, *submitted*

13. David Quinero, Alexey Kaledin, Aleksey E. Kuznetsov, Yurii, V. Geletii, Claire Besson, Craig L. Hill, Djameladdin G. Musaev, „Computational studies of the geometry and electronic structure of an all-inorganic and homogeneous tetra-Ru-polyoxometalate catalyst for water oxidation and its four one-electron oxidized forms“, *J. Phys. Chem. A.*, **2009**, *submitted*
14. Hui-Lung Chen, Hsin-Tsung Chen, Shin-Pon Ju, Djameladdin G. Musaev, M. C. Lin, „A Density-Functional theory study of the Adsorption and reaction of HCl and H₂O molecules over W(111) surfaces“, *J. Phys. Chem. C.* **2009**, *113*, *submitted*
15. Alexey L. Kaledin, Tianquan Lian, Yurii V. Geletii, Craig L. Hill, and Djameladdin G. Musaev, „Insights into photoinduced electron transfer between $[\text{Ru}(\text{bpy})_3]^{2+}$ and $\text{S}_2\text{O}_8^{2-}$ in water: computational and experimental studies“, *J. Phys. Chem. A.*, **2009**, *submitted*

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16. 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 Nadjjo, Djameladdin 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
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18. Jerzy Moc, Djameladdin G. Musaev, Keiji Morokuma, “Zeolite-Supported Palladium Tetramer and Its Reactivity toward H₂ Molecules: Computational Studies” *J. Phys. Chem. A.* **2008**, *112*, 5973-5983
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20. Hsin-Tsung Chen, Djameladdin 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.
21. Hsin-Tsung Chen, Jee-Gong, Chang, Djameladdin 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
22. 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
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26. Rui Cao, Jong Woo Han, Traves M. Anderson, Daniel A. Hillesheim, Martin L. Kirk, Djameladdin G. Musaev, Keiji 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.

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