

Publications

- (1) Arsalan Mirjafari, David Siegel, Rachel Burton, Joseph Muller, Matthew Regner, **Yinghong Sheng**, Gregory McManus, James MacDonald “From gene delivery agents to ionic liquids: The impacts of cation structure and anion identity on liquefaction”, *Journal of Molecular Liquids*, **2019**, 276, 334-337.
- (2) **Yinghong Sheng**, Matthew Regner “Role of Water Molecules and Counterion on HS⁻ Sensing Reaction Utilizing a Pyrylium Derivative: A Computational Study”, *J. Phys. Chem. A*, **2019**, 123, 3334-3343. (Featured in Cover of the journal)
- (3) Zack Schultz, Jamie C. Gaitor, Rachel D. Burton, Matthew Regner, **Yinghong Sheng**, Arsalan Mirjafari “Phosphorodithioate-functionalized ionic liquids: synthesis, physicochemical properties and palladium complexation studies” *J. Mol. Liq.* **2019**, 276, 334-337.
- (4) Jinghui Li, Huaya Zheng, Wei Wang, Yubin Miao, **Yinghong sheng** and Changjian Feng “Role of an isoform-specific residue at the calmodulin-heme (NO synthase) interface in the FMN – heme electron transfer” *FEBS Letters* **2018**, 592, 2425-2431.
- (5) Jamie C. Gaitor, Lauren M. Paul, Melissa M. Reardon, Taha Hmissa, Samuel Minkowicz, Matthew Regner, **Yinghong Sheng**, Scott F. Michael, Sharon Isern and Arsalan Mirjafari “Ionic liquids with thioether motifs as synthetic cationic lipids for gene delivery” *Chem. Commun.*, **2017**, 53, 8328. (Cover Article Candidate)
- (6) S. Thigpen, S. T. Nestor, R. A. O’Brien, S. Minkowicz, **Y. Sheng**, J. H. Davis, Jr., K. N. West, A. Mirjafari, “Thioether-functionalized picolinium ionic liquids: synthesis, physical properties and computational studies”. *New Journal of Chemistry*, **2017**, 41, 1625-1630.
- (7) O'Brien, Richard A.; Zayas, Manuel Sanchez; Nestor, Stephen T.; Gaitor, Jamie C.; Paul, Lauren M.; Edhegard, Forrest A.; Minkowicz, Samuel; Sykora, Richard E.; **Sheng, Yinghong**; Michael, Scott F.; Isern, Sharon; Mirjafari, Arsalan, “Correction: Biomimetic design of protic lipidic ionic liquids with enhanced fluidity” *New Journal of Chemistry* **2016**, 40, 8970.
- (8) O'Brien, Richard A.; Zayas, Manuel Sanchez; Nestor, Stephen T.; Gaitor, Jamie C.; Paul, Laurant M.; Edhegard, Forrest A.; Minkowicz, Samuel; Sykora, Richard E.; **Sheng, Yinghong**; Michael, Scott F.; Isern, Sharon; Mirjafari, Arsalan, “Biomimetic design of protic lipidic ionic liquids with enhanced fluidity” *New Journal of Chemistry* **2016**, 40, 7795 – 7803.
- (9) O'Brien, Richard A.; Zayas, Manuel Sanchez; Nestor, Stephen T.; Gaitor, Jamie C.; Paul, Laurant M.; Edhegard, Forrest A.; Minkowicz, Samuel; Sykora, Richard E.; **Sheng, Yinghong**; Michael, Scott F.; Isern, Sharon; Mirjafari, Arsalan,

- [“CCDC 1450654: Experimental Crystal Structure Determination”](#), Cambridge Crystallographic Data Centre, **2016**.
- (10) Manuel Sanchez Zayas, Jamie C. Gaitor, Stephen T. Nestor, [Samuel Minkowicz](#), **Yinghong Sheng** and Arsalan Mirjafari, [“Bifunctional hydrophobic ionic liquids: Facile synthesis by thiol-ene “click” chemistry”](#) *Green Chemistry*, **2016**, 18, 2443–2452.
- (11) **Yinghong Sheng**, Linghao Zhong, Dahai Guo, [Gavin Lau](#), Changjian Feng, [“Insight into structural rearrangements and interdomain interactions related to electron transfer between flavin mononucleotide and heme in nitric oxide synthase: A molecular dynamics study”](#) *Journal of Inorganic Biochemistry* **2015**, 153, 186–196.
- (12) Richard A. Braun, Joseph L. Bradfield, Codey B. Henderson, Niloufar Mobarrez, **Yinghong Sheng**, Richard A. O’Brien, Alexandra C. Stenson, James H. Davis Jr. and Arsalan Mirjafari, [“Click chemistry mediated synthesis of bio-inspired phosphonyl-functionalized ionic liquids”](#) *Green Chem.*, **2015**, 17, 1259-1268.
- (13) **Yinghong Sheng**, Jerzy Leszczynski, [“Thermal racemization of spiropyrans: implication of substituent and solvent effects revealed by computational study”](#), *Struct. Chem.* **2014**, 25, 667-677.
- (14) **Yinghong Sheng***, Yi Ren, “Computational Study on a HS⁻ Sensing Reaction Utilizing a Pyrylium Derivative”, *J. Phys. Chem. A*, **2012**, 116, 5420–5427.
- (15) Zhe Quan, Christine Purser, Rodney C. Baker, Terry Dwyer, Rajesh Bhagat, **Yinghong Sheng**, Jerzy R. Leszczynski, [“Determination of Derivatized Urea in Exhaled Breath Condensate by LC-MS”](#), *Journal of Chromatographic Science*, **2010**, 48, 140.
- (16) **Yinghong Sheng***, Heather D. Bean, [Irena Mamajanov](#), Nicholas V. Hud and Jerzy Leszczynski, [“Comprehensive Investigation of the Energetics of Pyrimidine Nucleoside Formation in a Model Prebiotic Reaction”](#), *J. Am. Chem. Soc.* **2009**, 131, 16088.
- (17) Chao Deng, [Xiao-Peng Wu](#), [Xiao-Ming Sun](#), Yi Ren, **Ying-Hong Sheng*** [“Neutral hydrolyses of carbon disulfide: An ab initio study of water catalysis”](#), *J. Comput. Chem.* **2009**, 30, 285.
- (18) [Min Yu](#), Marek. W. Urban, **Yinghong Sheng**, Jerzy, Leszczynski [“Molecular Recognition at Methyl Methacrylate/n-Butyl Acrylate \(MMA/nBA\) Monomer Unit Boundaries of Phospholipids at p-MMA/nBA Copolymer Surfaces”](#), *Langmuir*, **2008**, 24, 10382.
- (19) [Heather D. Bean](#), **Yinghong Sheng**, James P. Collins, Jerzy Leszczynski, and Nicholas V. Hud [“Formation of a \$\beta\$ -Pyrimidine Nucleoside by a Free Pyrimidine Base and Ribose in a Plausible Prebiotic Reaction”](#), *J. Am. Chem. Soc. Communications*. **2007**, 129, 9556.

- (20) **Yinghong Sheng**, Jerzy Leszczynski, Thuc-Quyen Nguyen, Anu Bamgbelu “Theoretical Study on the Structure and Property Relationship of the Cationic Conjugated Polyelectrolytes”, *Structural Chemistry*, **2007**, 18, 827.
- (21) **Shuguang Wang**, **Yinghong Sheng**, Manliang Feng, Lei Wang, Jerzy Leszczynski, Hiroyasu Tachikawa, and Hongtao Yu “Light-Induced Cytotoxicity of 16 Polycyclic Aromatic Hydrocarbons on the US EPA Priority Pollutant List in Human Skin HaCaT Keratinocytes: Relationship between Phototoxicity and Excited State Properties”, *Environmental Toxicology*, **2007**, 22(3), 318-327.
- (22) **Yinghong Sheng**, Jerzy Leszczynski “Theoretical Study of the Regioselectivity of the Cycloaddition Reaction between Cyclopentadiene and Methyleneketene”, *Tetrahedron*, **2006**, 62(29), 7014.
- (23) **Yinghong Sheng**, Szczepan Roszak, and Jerzy Leszczynski, “The Molecular Structures and Nature of Interactions in $N_2H^+-He_n$ ($n = 1 - 12$) Complexes”, *Mol. Phys.* **2005**, 103, 1091.
- (24) Zhe Quan; Yaru Song; Andrea Saulsberry; **Yinghong Sheng**; Yi-Ming Liu. “Capillary Electrophoresis for Diastereomers of (R,S)-Tetrahydroisoquinoline-3-Carboxylic Acid Derivatized with (R)-4-Nitro-7-(3-Aminopyrrolidin-1-yl)-2,1,3-Benzoxadiazole: Effect of Molecular Geometries.” *Journal of Chromatographic Science*, **2005**, 43(3), 121-125.
- (25) Zhe Quan, Yaru Song, Gladys Peters, Ming Shengwu, **Yinghong Sheng**, Huey-Min Hwang, and Yi-Ming Liu, “Chiral CE Separation of Dopamine Derived Neurotoxins”, *Analytical Sciences*, **2005**, 21(2), 115-9.
- (26) **Yinghong Sheng**, Szczepan Roszak, and Jerzy Leszczynski, “Microsolvation of N_2H^+ : The nature of interactions in $N_2H^+-(H_2)_n$ ($n = 1 - 14$) complexes”, *J. Chem. Phys.*, **2004**, 120, 4324.
- (27) **Yinghong Sheng**, Yun-Dong Wu, Jerzy Leszczynski, “A Theoretical Study of the Ring-Opening of Metallacyclobutene Derived from the Addition of Acetylene to Molybdenum Alkylidenes”, *Organometallics*, **2004**, 23, 3189.
- (28) **Yinghong Sheng**, Jerzy A. Leszczynski, Antonio A. Garcia, Rohit Rosario, Devens Gust, Joseph Springer, “Comprehensive Theoretical Study of the Conversion Reactions of Spiropyran: Substituent and Solvent Effects”, *J. Phys. Chem. B*, **2004**, 108, 16233.
- (29) **Yinghong Sheng** and Jerzy Leszczynski, “Theoretical Study of the Substituent and Solvent Effects on the Molecular Structures, Absorption and Emission Spectra of Spiropyran” *Collection of Czechoslovak Chemical Communications*, **2004**, 69, 47-62.
- (30) **Yinghong Sheng**, Ramaiyer Venkatraman, Józef S. Kwiatkowski, Joanna Majewska and Jerzy Leszczynski, “A DFT and MP2 Study on the Molecular Structure, Vibrational Raman and Infrared Spectra of Halogenosubstituted Phosphoryl and Thiophosphoryl Compounds”, *Structural Chemistry*, **2003**, 20, 511.

- (31) **Yinghong Sheng** and Jerzy Leszczynski, "A Comprehensive Computational Study on $\text{OCH}^+\text{-Rg}$ ($\text{Rg} = \text{He, Ne, Ar, Kr, Xe}$) Complexes", *Collection of Czechoslovak Chemical Communications*, **2003**, 68, 489.
- (32) **Yinghong Sheng**, Djameladdin G. Musaev, Frank, E. McDonald and Keiji Morokuma, "Computational Studies of Tungsten-Catalyzed *endo*-Selective Cycloisomerization of 4-Pentyn-1-ol", *J. Am. Chem. Soc.*, **2002**, 124, 4149.
- (33) **Yinghong Sheng**, Robert W. Gora, Malgorzata Kaczorowska, Szczepan Roszak, and Jerzy Leszczynski, "The molecular structures, energetics, and nature of interactions in $\text{Ar}_n\text{-N}_2\text{H}^+$ ($n=1-12$) complexes", *J. Phys. Chem.*, **2002**, 106, 11162.
- (34) **Yinghong Sheng** and Jerzy Leszczynski, "A Comprehensive Computational Study of $\text{N}_2\text{H}^+\text{-X}$ ($\text{X} = \text{He, Ne, Ar, Kr, Xe, and H}_2$) Complexes", *J. Phys. Chem.*, **2002**, 106, 12095.
- (35) **Ying-Hong Sheng**, Yun-Dong Wu, "Theoretical Studies on Acetylene Addition to Molybdenum Alkylidenes: The preference of α - and β additions", *J. Am. Chem. Soc.*, **2001**, 123, 6662.
- (36) **Ying-Hong Sheng**, De-Cai Fang, Yun-Dong Wu, Xiao-Yuan Fu, Yuansheng Jiang, "DFT Study on the Mechanism of the Cycloaddition Reaction between Methylene ketene and 1-pyrroline-1-oxide", *Journal Molecular Structure: THEOCHEM*, **1999**, 467, 31.
- (37) **Ying-Hong Sheng**, De-Cai Fang, Yun-Dong Wu, Xiao-Yuan Fu, Yuansheng Jiang, "DFT Study on the Mechanism of the Cycloaddition Reaction between Methylene ketene and 5-Methylene-1,3-Dioxan-4,6-Dione: Solvent Effect and Regioselectivity", *Journal Molecular Structure: THEOCHEM*, **1999**, 488, 187-194.
- (38) **Yinghong Sheng**, Yuansheng Jiang, "Theoretical Study on Molecular First-Order Hyperpolarizability for Push-Pull Polyenes and Quinones: The Effects of Donor-Acceptor Pairs and Solvents", *Bulletin of the Chemical society of Japan*, **1999**, 72, 2155.
- (39) **Yinghong Sheng**, Yuansheng Jiang, Xiao-Chuan Wang, "An AM1 study of the relationship between the donor-acceptor strength and the polarizabilities of push-pull polyenes", *J. Chem. Soc. Faraday Trans.*, **1998**, 94, 47.
- (40) **Yinghong Sheng**, Yuansheng Jiang, "AM1/CI Study on the First-Order Hyperpolarizability of Push-Pull Polyenes and Push-Pull Quinones. A Two-Level Model Evaluation", *J. Chem. Soc. Faraday Trans.*, **1998**, 94, 1823.
- (41) **Yinghong Sheng**, Yuansheng Jiang, "Polarizability and Hyperpolarizability of Push-Pull Quinonoid Molecules: Simulation of Donor-Acceptor Pairs", *J. Chem. Soc. Faraday Trans.*, **1998**, 94, 1829.
- (42) **Yinghong Sheng**, Decai Fang, Xiaoyuan Fu, "Theoretical Study on the Mechanism of the Cycloaddition Reactions between Methylene ketene and 5-methylene-1,3-dioxan-4,6-dione", *Acta Physico-Chimica Sinica*, **1996**, 12, 496.

- (43) **Yinghong Sheng**, Decai Fang, Xiaoyuan Fu, "A Theoretical Study on the Mechanism of the Cycloaddition Reaction between Methyleneketene and 1-Oxo-Butadiene", *Journal of Beijing Normal University (Natural Science)*, **1995**, 31, 99.
- (44) **Yinghong Sheng**, Decai Fang, Xiaoyuan Fu, *The Seventh National Symposium on Physical Organic Chemistry of China*. Pp201-202, Xi'an, Oct. 10-20, **1995**.
- (45) Book Chapter in *Xin Xing Xue Ke Bai Wan Ge Wei Shen Me*, Center National University, **1994**.