

Yi-Gui Wang, Ph. D.

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Education

Postdoctoral associate, **Yale University**, Physical Organic Chemistry, (2002,7—2007,12)

Postdoctoral associate, **McMaster University**, Canada, Physical Organic Chemistry, (2000-2002)

Guest scientist, **Max-Planck Institute for the Physics of Complex Systems**, Germany,
Quantum Chemistry, (1998,8 --- 2000, 8)

Ph.D., Physical Chemistry (1998), Shandong University, P. R. China

M.S., Organic Chemistry (1993), Shandong University, P. R. China

B.S., Chemistry (1990), Shandong University, P. R. China

Academic Employment

Adjunct staff at University of New Haven (since January 2012)

Teach Physical Chemistry I & II Labs (CHE 333, CHE 334)
and General chemistry Lab (CH1106L)

Adjunct professor at Southern Connecticut State University (SCSU) (since September 2009)

- Teach Physical Chemistry I lecture (CHE 370, fall-2012. Fall 2014)
- Teach Physical Chemistry I & II labs (CHE 372, fall-2012. Fall 2014, Spring 2015)
- Instruct five sections of che-120 labs and five che-121 labs (General Chemistry I & II)
- Instruct six sections of che-125 labs (Introduction to General, Organic, and Biochemistry)
- Instruct six sections of CHE 101 labs (Chemistry in Context—Applying Chemistry to Society)
- Instruct two sections of CHE 103 labs (Forensic Chemistry)
- Prepared and supervised Forensic Test at Yale university science Olympiad (2015)
- judge for CT state science Olympiad at UCONN (2015, 2016)

Awards and Honors

Obtain “start-up” allocations on XSEDE supercomputers

Project : *ab initio studies on the glycosidation of 5-fluorouracil*
(June 2014, renewed June 2015)

and received allocations on more resources on December 21, 2015)

received research allocation on XSEDE supercomputers

Project: *ab initio studies on physical and chemical properties*

(January 1 2016-December 31, 2016; Renewed, Jan. 1, 2017—Dec. 31, 2017)

2015 David Csejka Award outstanding part-time faculty member at SCSU

Max Planck Institute scholarship, Max-Planck Institute for the Physics of complex systems
(1998-2000)

GUANGHUA scholarship, Shandong University, China (1993)

Outstanding Ph. D student (1998)

Affiliations

American chemical society

AAAS

Publication List

At SCSU

- 3) Wang, Y. G.; Barnes, E.
ZnCH₂ and HZnCH—Bonding Characteristics and Their Interconversion
In preparation 2017.
- 2) Wang, Y. G.; Barnes, E.
Theoretical Studies of the Glycosidation of 2-*O*-substituted 5-Fluorouracil:
O-Regioselective synthesis with the silver salt method
J. Org. Chem. **In Revision 2017.**
- 1) Wang, Y.G.; Barnes, E.
Theoretical studies of the glycosidation of 2-*O*-substituted 5-fluorouracil.
N-Regioselective synthesis with the phase-transfer-catalysis method
J. Phys. Chem. **Submitted Revision 2017.**

At Yale University, USA

PUBLICATIONS

- 19) Wiberg, K. B.; Caricato, M.; Wang, Y.G.; Vaccaro, P. H.
Towards the Accurate and Efficient Calculation of Optical Rotatory Dispersion Using
Augmented Minimal Basis Sets
Chirality, **2013**, *25(10)*, 606-616.
- 18) Wiberg, K. B.; Wang, Y. G.
A Comparison of Some Properties of C=O and C=S Bonds,
ARKVOC, **2011 (v)**, 45-56.
- 17) Wang, Y-G.
Examination on DFT and TDDFT Methods II
J. Phys. Chem. A **2009**, *113*, 10873.
- 16) Wang, Y-G.
Examination on DFT and TDDFT Methods I
J. Phys. Chem. A **2009**, *113*, 10867.
- 15) Rossi, A. R.; Wang, Y-G., Wiberg, K. B.
Excited States and Photochemistry of Bicyclo[1.1.0]butane.
J. Phys. Chem. A **2009**, *113(9)*, 1686.

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- 14) Wiberg, K. B.; Wang, Y.-G.; Miller, S. J.; Puchlopek, A. L. A.; Bailey, W. F.; Justin, J. D.
Disparate Behavior of Carbonyl and Thiocarbonyl Compounds: Acyl Chlorides vs
Thiocarbonyl Chlorides and Isocyanates vs Isothiocyanates.
J. Org. Chem. **2009**, *74*(10), 3659.
- 13) Wiberg, K. B.; Wang, Y.-G.; Petersson, G. A.; Bailey, W. F.
Intramolecular Nonbonded Attractive Interactions: 1-Substituted Propenes
J. Chem. Theory Comput. **2009**, *5*(4), 1033.
- 12) Wiberg, K. B.; Wang, Y.-G.; Wilson, S. M.; Vaccaro, P. H.; Jorgensen, W. L.; Crawford, T. D.
Cheeseman, J. R.; Luderer, M.
Chiroptical Properties of 2,3-Hexadiene and 2,3-Pentadiene
J. Phys. Chem. A. **2008**, *112*, 2415.
- 11) Wang, Y.-G.; Wiberg, K. B.; Werstiuk, N. H.
Correlation Effects in EOM-CCSD for the excited states: evaluated by AIM
localization Index (LI) and Delocalization Index (DI)
J. phys. Chem. A **2007**, *111*, 3592.
- 10) Wiberg, K. B.; Wilson, S. M.; Wang, Y.-G.; Vaccaro, P. H.; Cheeseman, J. R.; Luderer, M. R.
Effect of Substituents and Conformations on the Optical Rotations of Cyclic Oxides and
Related Compounds. Relationship between the Anomeric Effect and Optical Rotation.
J. Org. Chem. **2007**, *72*, 6206.
- 9) Wiberg, K. B.; Wang, Y.-G.; Sklenak, S.; Deutsch, C.; Trucks, G.
Permanganate Oxidation of Alkenes. Difficulties with MP2 Calculations
J. Am. Chem. Soc. **2006**, *128*, 11537.
- 8) Wiberg, K. B.; Wang, Y.-G.; Wilson, S. M.; Vaccaro, P. H.; Cheeseman, J. R.
Sum-over-States Calculation of the Specific Rotations of Some Substituted Oxiranes,
Chloropropionitrile, Ethane and Norbornenone,
J. Phys. Chem. A. **2006**, *110*, 13995.
- 7) Wiberg, K. B.; Wang, Y.-G.; Wilson, S.; Vaccaro, P. H.; Cheeseman, J. R.
Chiroptical Properties of 2-Chloropropionitrile
J. Phys. Chem. A. **2005**, *109*, 3448.
- 6) Wiberg, K. B.; Wang, Y.-G.; Vaccaro, P. H.; Cheeseman, J. R.; Luderer, M. R.
Conformation Effects on Optical Rotation. 2-Substituted Butanes
J. Phys. Chem. A. **2005**, *109*, 3405.
- 5) Wiberg, K. B.; Wang, Y.-G.; de Oliveira, A. E.; Perera, A.; Vaccaro, P. H.
Comparison of CIS and EOM-CCSD Calculated Adiabatic Excited State Structures.
Changes in Density from Ground States to Excited States.
J. Phys. Chem. A. **2005**, *109*, 466.

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- 4) Wiberg, K. B.; Wang, Y.-G.; Vaccaro, P. H.; Cheeseman, J. R.; Trucks, G.; Frisch, M. J.
Optical activity of 1-butene, butane and related hydrocarbons
J. Phys. Chem. A **2004**, *108*, 32.
- 3) Wiberg, K. B.; Wang, Y.-G.
Conformational Energies for 2-Substituted Butanes
J. Comput. Chem. **2004**, *25*, 1127.
- 2) Wiberg, K. B.; Wang, Y.-G.; Murphy, M. J.; Vaccaro, P. H.
Temperature Dependence of the Optical Rotation: α -Pinene, β -Pinene, Pinane,
Camphene, Camphor and Fenchone
J. Phys. Chem. A **2004**, *108*, 5559.
- 1) Wiberg, K. B.; Wang, Y.-G.
Electronic excited states for methylenecycloalkane
J. Phys. Chem. A **2004**, *108*, 9417.

PRESENTATIONS

- 1) Wiberg, K. B.; Wang, Y.-G.; de Oliveira, A. E.; Perera, A.; Vaccaro, P. H.
Comparison of CIS and EOM-CCSD Calculated Adiabatic Excited State Structures.
(Oral presentation) Quantum chemistry meeting of Connecticut, **February, 2004**
- 2) Wang, Y.-G.; Wiberg, K. B. Conformational Effects on the Optical Rotation,
(Poster), 2005 Gordon Research Conference of Physical Organic Chemistry, New Hampshire.
June, 2005.
- 3) Wang, Y.-G.; Wiberg, K. B.
Optical activity of 2,3-hexadiene,
(Oral presentation) Quantum chemistry meeting of Connecticut, **February, 2006**

OTHERS

- 1) Wiberg, K. B.; Wang, Y.-G.; Trucks, G.; Frisch, M. J.
Effect of DFT Model on Calculated Ground State Properties
to be submitted.
- 2) Wiberg, K. B.; Wang, Y.-G.
A Reexamination of Substituted Effects of Benzene
to be submitted

At McMaster University, Canada

PUBLICATIONS

- 1) Wang, Y.-G.; Werstiuk, N. H.
A Practical and efficient method to calculate AIM localization and delocalization indices at post-HF levels of theory
J. Comput. Chem. **2003**, *24*(3), 379.
- 2) Wang, Y.-G.; Matta, C. F.; Werstiuk, N.H.
A comparison of localization and delocalization indices obtained with Hartree-Fock and conventional correlation methods: the effect of Coulomb correlation
J. Comput. Chem. **2003**, *24*, 1720.
- 3) Wang, Y.-G.; Matta, C. F.; Werstiuk, N.H.
A comparison of localization and delocalization indices obtained with Hartree-Fock and conventional correlation methods: the effect of Coulomb correlation
J. Comput. Chem. **2004**, *25*, 309.
- 4) Werstiuk, N.H.; Wang, Y.-G.
An Atoms in Molecules and Electron Localization Function Computational Study on the Structure of the 6-Tricyclo[3.2.1.0^{2,4}] octyl Cation.
J. Phys. Chem. A. **2001**, *105*, 11515.
- 5) Werstiuk, N.H.; Wang, Y.-G.
Creating three penta-coordinated carbons in a six-member ring. An AIM and ELF study Of the Trishomocyclopropenyl cation and phosphorus, sulfur, arsenic, and selenium analogues
J. Phys. Chem. A **2003**, *107*, 9434.
- 6) Werstiuk, N.H.; Wang, Y.-G.
A Density Functional Theory (DFT) study on the 6-tricyclo[3.2.1.0^{2,4}]octyl cation and its isomers: a walk on the C₈H₁₁⁺ potential energy surface.
ARKIVOC, **2001**, *12*, 187.

PRESENTATIONS

- 1) Wang, Y.-G.; Werstiuk, N.H.
AIM and ELF Studies on the Topological Properties of the Electron Density of CH₃-CH₃, LiF and NH₃BH₃
29th Ontario - Quebec Physical Organic mini-Symposium, Poster
- 2) Werstiuk, N.H.; Wang, Y.-G.
The structure of protonated cyclopropane: AIM and ELF studies
29th Ontario - Quebec Physical Organic mini-Symposium, Poster

At Max-Planck Institute for the Physics of the Complex Systems (MPIPKS-dresden, Germany)

PUBLICATIONS

- 1) Wang, Y.-G.; Dolg, M.; Bian, W.-S.; Deng, C.-H.
Ab initio study of the reaction mechanism of CH^{3+} and CH^{3-} with $\text{CH}_2=\text{CNa}(\text{OH})$
Journal of Physical Chemistry A **1999**, 103(18), 3472.
- 2) Wang, Y.-G.; Dolg, M.
Theoretical Confirmation of the Stereoselectivity in the Reverse Brook Rearrangement
Tetrahedron **1999**, 55(44), 12751.
- 3) Wang, Y.-G.; Sun, C.-J.; Bian, W.-S.; Deng, C.-H.
Ab initio study of $\text{MCH}_2(\text{OH})$ and $\text{CH}_3\text{OM}(\text{M}=\text{H}, \text{-}, \text{Li}, \text{Na})$
Chemical Research In Chinese Universities-English, **2000**, 16(2), 136.

PRESENTATIONS

Theoretical Confirmation of the Stereoselectivity in the Reverse Brook Rearrangement (poster) 35th symposium for theoretical chemistry, Freiberg, Germany, 1999.

OTHERS

- 1) Wang, Y.-G.; Kohout, M.
Why dimethyl ether cleavages via a carbenoid mechanism
to be submitted
- 2) Wang, Y.-G.
The reactivity and the structure of saturated carbenoid H_2CMX ($\text{M}=\text{-}, \text{Li}$; $\text{X}=\text{N}, \text{P}, \text{As}$; $\text{O}, \text{S}, \text{Se}$; $\text{F}, \text{Cl}, \text{Br}$): a high level study
- 3) Wang, Y.-G.
The reactivity and the structure of un-saturated carbenoid $\text{H}_2\text{C}=\text{CMX}$ ($\text{M}=\text{-}, \text{Li}$; $\text{X}=\text{N}, \text{P}, \text{As}$; $\text{O}, \text{S}, \text{Se}$; $\text{F}, \text{Cl}, \text{Br}$): a high level study
- 4) Wang, Y.-G.; Pleutin, S.; Birkenheue, U.
ab initio Studies on Materials with Carbon Kink Chain
- 5) Wang, Y.-G.; Birkenheuer, U.; Bottcher, P.
 Se_8 ring: Novel Structure in $\text{Gd}_8\text{Se}_{15}$ Crystals

Ph. D. work at Shandong University

- 1) Wang, Y.-G.; Sun, C.-J.; Deng, C.-H.
A theoretical study of C_2H_3ONa
Journal of Physical Chemistry A, **1998**, 102(29), 5816.
- 2) Wang, Y.-G.; Sun, C.-J.; Deng, C.-H.
A theoretical study of C_2H_3OLi
THEOCHEM-Journal of Molecular Structure, **1998**, 429, 207.
- 3) Li, S.-L.; Wang, Y.-G.; Chen, S.-H. et al.
Some aspects of quantum chemical calculations for the study of Schiff base corrosion inhibitors on copper in NaCl solutions
Corrosion Science, **1999**, 41(9), 1769.
- 4) Bian, W.-S.; Zhao, X.; Wang, Y.-G.; Wang, Y.-X.; Deng, C.-H.
Direct solution of the Schrodinger equation for some muonic molecules
Chemical Physics, **1999**, 242(2), 195.
- 5) Wang, Y.-G.; Sun, C.-J.; Deng, C.-H.
Ab initio studies on reaction $H_2C = C(OH)Li + CH_3^+(CH_3)$
Science in China Series B, **1998**, 41(6), 587.
- 6) Wang, Y.-G.; Sun, C.-J.; Deng, C.-H.
Theoretical studies of acyl reagents with Umploung central carbon - II.
A theoretical study of $CH_2 = C(OH)Na$
Huaxue Xuebao, **1998**, 56(9), 840.
- 7) Wang, Y.-G.; Sun, C.-J.; Deng, C.-H.
Ab initio studies of lithium ethenolate
Gaodeng Xuexiao Huaxue Xuebao, **1998**, 19(3), 424.
- 8) Wang, Y.-G.; Sun, C.-J.; Cai, Z.-T.; Deng, C.-H.
Ab initio study on alkali metal enolates $CH_2=CH(OM)$
Wuli Huaxue Xuebao, **1999**, 15(2), 116.
- 9) Wang, Y.-G.; Sun, C.-J.; Li, H.-X.; Deng, C.-H.
An ab initio study on sodium ethenolate,
Fenzi Kexue Xuebao, **1999**, 15(2), 91.
- 10) Wang, Y.-G.; Sun, C.-J.; Deng, C.-H.
An ab initio study on $CH_2=CH(XM)$ ($X=S, Se, Te$; $M=H, Li, Na, K, Rb, Cs$)
Fenzi Kexue Xuebao, **1998**, 14(4), 215.

Work before Ph. D. degree

- 1) Sun, C.-J.; Li, H.-X.; Li, J.-H.; Wang, Y.-G.; Qi, Y.-X.; Zhang, J.-M.; Liu, S.-Y.
Synthesis of 2-substituted 3-acyl-5-fluoro-4-pyrimidinones and their antitumor activities.
Hecheng Huaxue, **2000**, 8(3), 248.
- 2) Sun, C.-J.; Xue, J.; Wang, Y.-G.; Li, H.-X. et al.
Synthesis of 5-fluorouracil derivatives and their antitumor activities.
Zhongguo Yaowu Huaxue Zazhi, **1998**, 8(2), 91.
- 3) Sun, C. -J.; Li, H.-X.; Qi, Y.X.; Wang, Y.-G.; Zhang, J.M.; Jiao, X.H
Study on synthesis of 2,3-disubstituted-5-fluorouracils and their antitumor activities.
Hecheng Huaxue, **1997**, 5(3), 221. (cited 1 time)
- 4) Sun, C.-J.; Wang, Y.-G.; Qi, Y.-X. et al.
Method for synthesis of 2-aryloxy-5-fluoro-3H-4-pyrimidone.
Hecheng Huaxue, **1997**, 5(1), 61.
- 5) Lin, J.-M.; Wang, B.; Liu, Y.-Y.; Wang, Y.-G.; Ma, Y.-D.
Synthesis of some new gamma-N-[(arylidene-aminoethyl)aminoethyl]aminopropyl
-2,8,9-trioxa-5-aza-1-silabicyclo[3,3,3]undecanes
Synthetic Communications, **1997**, 27(24), 4309.
- 6) Sun, C.-J.; Sun, Y.; Wang, Y.-G.; Li, H.-X.; et al
Synthesis of glycosides (VII). Synthesis of glycosides of 1-arylsulonyl-5-fluorouracils
and their antitumor activities.
Shandong Daxue Xuebao, Ziran Kexueban, **1997**, 32, 443.
- 7) Sun, C.-J.; Wang, Y.-G.; Li, H.-X. et al.
Synthesis of glycosides(IX). Synthesis of beta-D-xylopyranosides of 5-fluoro
-uracil and their antitumor activities,
Zhongguo Yaowu Huaxue Zazhi, **1997**, 7(2), 84.
- 8) Sun, C.-J.; Wang, Y.-G.; Li, H.-X. et al.
Synthesis of glycosides(VII). Synthesis of methyl 1-O-arylcarbonyl-2,3,4-tri
-O-acetyl-beta-D-glucopyranuronate and their antitumor activities.
Shandong Daxue Xuebao, Ziran Kexueban, **1996**, 31(3), 327.
- 9) Sun, C.-J.; Wang, Y.-G.; Li, H.-X. et al.
Synthesis of glycosides(VI). Synthesis of 1-O-beta-D-(5-substituted-2-furoyl
)-acetyl-gluco and xylo-pyranose and their antitumor activities.
Zhongguo Yaowu Huaxue Zazhi, **1996**, 6(3), 162.

- 10) Sun, C.-J.; Wang, Y.-G.; Li, H.-X. et al.
The preparation of 1-O-beta-D-(5-substituted-2-furoyl)-acetylated sugars by phase transfer catalysis.
Hecheng Huaxue, **1996**, 4(1), 5.
- 11) Sun, C.-J.; Li, H.-X.; Wang, Y.-G.; Qi, Y.-Y. et al.
A new method of preparing 3-N-substituted-5-fluorouracils,
Hecheng Huaxue, **1996**, 4, 293.
- 12) Sun, C.-J.; Wang, Y.-G.; Li, H.-X. et al.
The synthesis of beta-D-xylopyranosides of 2-substituted-5-fluorouracil.
Hecheng Huaxue, **1996**, 4(3),195.
- 13) Sun, C.-J.; Wang, Y.-G.; Chen, Z.-C. et al.
Synthesis of N-glucuronides of 5-fluorouracil and their antitumor activities,
Chinese Chemical Letters, **1994**, 5(5), 375.
- 14) C.-J. Sun, Y.-G. Wang, Z.-C. Chen, et al.
Synthesis of glycosides(V). Sythesis of O-glucuronides of 2-O-ackyl-5-fluoro-uracils and their antitumor activities.
Hecheng Huaxue, **1994**, 2(3), 246.
- 15) Sun, C.-J.; Wang, Y.-G.; Chen, Z.-C. et al.
Synthesis of glycosides(IV). Sythesis of N-glucuronides of 5-fluoro-uracils and their antitumor activities.
Gaodeng Xuexiao Huaxue Xuebao, **1994**, 15(8), 1168.
- 16) Sun, C.-J.; Chen, Z.-C.; Meng, Y.; Wang, Y.-G.; Xue, P. et al.
Synthesis of 2-alkoxy-5-fluoro-3H-4-Pyrimidones.
Shandong Daxue Xuebao, Ziran Kexueban, **1994**, 29, 192.
- 17) Sun, C.-J.; Chen, Z.-C.; Wang, Y.-G.; Xue, P.
Studies on the synthesis of D-glucuronic acid derivatives of 2-butoxy-fluoro-3H-4-Pyrimidones and their anticancer activities.
Chinese chemical letters, **1993**, 4, 197.
- 18) Sun, C.-J.; Chen, Z.-C.; Zhang, Y.-N.; Wang, Y.-G.; Zhang, C.-R.
Synthesis of galactopyrnsides of 5-fluorouracil
Youji Huaxue, **1992**, 12, 273.